=>

Uploading C:\Program Files\Stnexp\Queries\10552382-broad.str

chain nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-2 1-3 1-4 1-5 5-6 5-10 6-7 7-8 7-9

exact/norm bonds :

1-2 1-3 1-4 1-5 5-6 5-10 6-7 7-8 7-9

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:CLASS

Generic attributes :

Saturation : Saturated

#### STRUCTURE UPLOADED L1

FILE 'REGISTRY' ENTERED AT 06:32:41 ON 19 MAY 2008

STRUCTURE UPLOADED L1

1 S L1 L2

157 S L1 SSS FULL L3

FILE 'CAPLUS' ENTERED AT 06:33:09 ON 19 MAY 2008

59 S L3

L52 S US200!-552382/APPS

L6 1 S L4 AND L5

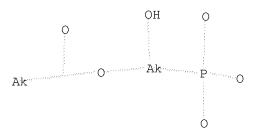
L7 58 S L4 NOT L5

FILE 'REGISTRY' ENTERED AT 06:33:31 ON 19 MAY 2008

=> d 11

L1 HAS NO ANSWERS

L1STR



Structure attributes must be viewed using STN Express query preparation.

```
ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
1.6
      ΑN
DN
      141:366424
      Preparation of analogs of lyso-phosphatidic acid as potential antitumor,
TI
      anti-inflammatory, and antidiabetic agents
ΙN
      Prestwich, Glenn D.; Xu, Yong; Qian, Lian
      University of Utah Research Foundation, USA
PA
      PCT Int. Appl., 145 pp.
SO
      CODEN: PIXXD2
DT
      Patent
      English
LA
FAN.CNT 1
      PATENT NO.
                             KIND
                                                    APPLICATION NO.
                                       DATE
                                                                                 DATE
      _____
                              ____
                                       _____
                                                     ______
      WO 2004092188
                              A2
                                       20041028
                                                     WO 2004-US11060
                                                                                 20040409
PΙ
                              А3
      WO 2004092188
                                       20050428
           W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
                CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
               GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
          NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
                SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
                TD, TG
                                                                                 20040409
      EP 1615937
                                       20060118
                                                    EP 2004-749962
                               Α2
          R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
                                                    US 2006-552382
      US 20070123492
                              A1
                                      20070531
                                                                                 20060828 <--
                               Р
PRAI US 2003-462095P
                                       20030409
      WO 2004-US11060
                               W
                                       20040409
OS
      MARPAT 141:366424
GΙ
```

Described herein the preparation of analogs of lysophosphatidic acid I and II, AΒ wherein X1, X2, Y1, and Y2 comprises, independently, hydrogen, fluorine, a hydroxy group, alkyl, OR2, OCH2CH2OR2, OC(0)R3, or NC(0)R3; each U comprises, independently, oxygen, sulfur, or NR1; V is not present or when V is present, V comprises oxygen or sulfur; W comprises oxygen or sulfur; Z comprises oxygen, sulfur, NR1, CH2, CHF, CF2, or CHOR2; each R1 comprises, independently, hydrogen, alkyl, cationic counterion, or both R1 form a cyclic or heterocyclic group; R2 comprises hydrogen, alkyl, cycloalkyl, heterocycloalkyl, arvl, heteroaryl, protecting group; R3 is alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, Yland Y2 are different groups, the stereochem. at carbon a is either substantially R or substantially S, and wherein the compound having the formula I is not 1-acyl-sn-glycerol 3-phosphate and 2-acyl-sn-glycerol 3-phosphate, and wherein when V is not present, W is oxygen, X1 and Y1 are hydrogen, and X2 is hydroxy, then Y2 is not hydroxy. Also described herein are methods of making and using analogs of lysophosphatidic acid. Thus, cyclic phosphonate III was prepared as potential antitumor, anti-inflammatory, and antidiabetic agent (no data).

### => d 17 50-58 bib abs hitstr

L7 ANSWER 50 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1975:410634 CAPLUS <<LOGINID::20080519>>

DN 83:10634

OREF 83:1797a,1800a

TI Phosphorus-containing carbohydrates. XI. Synthesis of  $\alpha$ -hydroxyand  $\alpha$ -amino-phosphonates of acyclic monosaccharides

AU Paulsen, Hans; Kuhne, Helmut

CS Inst. Org. Chem. Biochem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.

SO Chemische Berichte (1975), 108(4), 1239-45 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

GI For diagram(s), see printed CA Issue.

AB 2,3:4,5-Di-O-isopropylidene-D-xylose reacted with (MeO)2HPO to give dimethyl 2,3:4,5-di-O-isopropylidene-D-xylitol 1-phosphonate. 2,3-O-isopropylidene-D-glyceraldehyde and 2,4-O-ethylidene-D-erythrose reacted with (MeO)2HPO to give 1:1 mixts. of the S- and R-α-hydroxyphosphonates. Treatment of 2,3:4,5-di-O-isopropylidene-D-arabinose with PhCH2NH2 gave the azomethine (I), which adds (MeO)2HPO followed by hydrogenation to give the crystalline D-arabinitol 1-phosphonate II.

RN 55644-20-7 CAPLUS

CN D-Galactitol, 1-C-(dimethoxyphosphinyl)-, 2,3,4,5,6-pentaacetate (CA INDEX NAME)

RN 55644-21-8 CAPLUS

CN D-Mannitol, 2-C-(dimethoxyphosphinyl)-, 1,3,4,5,6-pentaacetate (CA INDEX NAME)

Absolute stereochemistry.

RN 55722-28-6 CAPLUS

CN D-Glucitol, 2-C-(dimethoxyphosphinyl)-, 1,3,4,5,6-pentaacetate (9CI) (CA INDEX NAME)

L7 ANSWER 51 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1974:536404 CAPLUS <<LOGINID::20080519>>

DN 81:136404

OREF 81:21481a,21484a

TI Phosphorus-containing carbohydrates. IX. Synthesis of (1S)-dialkyl-D-arabitol-1-phosphonate and its derivatives

AU Paulsen, Hans; Kuhne, Helmut

CS Inst. Org. Chem. Biochem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.

SO Chemische Berichte (1974), 107(8), 2635-43 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

OS CASREACT 81:136404

GI For diagram(s), see printed CA Issue.

AB 2,3:4,5-Di-O-isopropylidene-D-arabinose reacted with HPO(OMe)2 to give 86% ester I, which was converted into partially blocked derivs., II via deblocking, and III (R = H) via periodate oxidation, resp. The configuration at C-1 of I was determined by NMR spectroscopy of the acyclic pentaacetate and the cyclic derivative III (R = Ac).

IT 53910-64-8P

RN 53910-64-8 CAPLUS

CN D-Arabinitol, 1-C-(dimethoxyphosphinyl)-, 2,3,4,5-tetraacetate, (S)- (9CI) (CA INDEX NAME)

L7 ANSWER 52 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1972:14713 CAPLUS <<LOGINID::20080519>>

DN 76:14713

OREF 76:2407a,2410a

TI 1,1-Ethanediphosphonic acids and their salts and esters

IN Kerst, Al F.

PA Monsanto Co.

SO Ger. Offen., 61 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	DE 2117880	A	19711028	DE 1971-2117880	19710413		
	US 3705191	A	19721205	US 1970-27988	19700413		
	NL 7104745	A	19711015	NL 1971-4745	19710408		
	FR 2089481	A5	19720107	FR 1971-12737	19710409		
	ES 390099	A1	19730601	ES 1971-390099	19710412		
	CA 986944	A1	19760406	CA 1971-110062	19710412		
	BE 765633	A1	19711013	BE 1971-102103	19710413		
	GB 1329879	A	19730912	GB 1971-26858	19710419		
	US 3816518	A	19740611	US 1972-234328	19720313		
	US 3846482	A	19741105	US 1972-283019	19720823		
	US 3846483	A	19741105	US 1972-283115	19720823		
	US 3890378	A	19750617	US 1972-283114	19720823		
PRAI	US 1970-27988	A	19700413				

AB A series of title compds. was prepared by addition of various reagents to 1,2-epoxy-1,1-ethanediphosphonic acid (I) or a salt or ester of I. Thus, reaction of I with H2O gave HOCH2C(OH)[P(O)(OH)2]2. I with liquid NH3 at -50° gave a mixture of H2NCH2C(OH)[P(O)(ONH4)2]2 and HOCH2C(NH2)[P(O)(ONH4)2]2. I tetra-Et ester, PrOH, and Na gave a mixture of PrOCH2C(OH)[P(O)(OEt)2]2 and HOCH2C(OPr)[P(O)(OEt)2]2. Other examples (16) were given.

IT 34619-93-7P 34619-94-8P

RN 34619-93-7 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)

RN 34619-94-8 CAPLUS

CN Phosphonic acid, [1-(acetyloxy)-2-hydroxyethylidene]bis- (9CI) (CA INDEX

NAME)

L7 ANSWER 53 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1971:488759 CAPLUS <<LOGINID::20080519>>

DN 75:88759

OREF 75:14065a,14068a

TI Antibiotic substituted phosphonic acids and salts

IN Christensen, Burton G.; Beattie, Thomas R.; Graham, Donald W.

PA Merck and Co., Inc.

SO Fr. Demande, 104 pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	FR 2034480		19710108	FR			
	US 3657282		19720418	US	19690123		
	US 3822296		19740702	US 1972-215917	19720106		
PRAI	US		19690123				

AB Title compds., useful as antibiotics, were prepared Thus, (iso-PrO)3P was added to epibromohydrin at 135° under N to give diiso-Pr 2,3-epoxypropylphosphonate. This (5 g) in 60 ml C6H6 was cooled to 3°, 2% tert-BuOK in tert-BuOH (8.8 ml) added under N at 3° to give 2.81 g di-iso-Pr trans-(3-hydroxypropenyl)phosphonate. This in concentrated HCl was refluxed under N 30 min to give trans-(3-hydroxypropenyl)phosphonic acid, which was epoxidized to give Na trans-(1,2-epoxy-3-hydroxypropyl)phosphonate. This passed through a cation exchange resin gave the free acid.

IT 34170-90-6P

RN 34170-90-6 CAPLUS

CN Phosphonic acid, [2-chloro-1-hydroxy-1-(hydroxymethyl)ethyl]-, diisopropyl ester, monoacetate (8CI) (CA INDEX NAME)

L7 ANSWER 54 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1971:436558 CAPLUS <<LOGINID::20080519>>

DN 75:36558

OREF 75:5793a,5796a

- TI Synthesis of carbohydrate derivatives with phosphorus-carbon bonds
- AU Zhdanov, Yu. A.; Uzlova, L. A.; Glebova, Z. I.
- CS Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR
- SO Doklady Akademii Nauk SSSR (1971), 197(6), 1331-4 [Chem] CODEN: DANKAS; ISSN: 0002-3264
- DT Journal
- LA Russian
- AB Keeping 2,3,4,5,6-penta-O-acetyl-aldehydo-D-galactose with (EtO)2PHO and a little Et3N 15 days gave 41% syrupy di-Et 1-hydroxy-D-galacto-2,3,4,5,6-pentaacetoxyhexylphosphonate. Similarly were prepared 5 addnl. phosphonates. Treating the chloride of penta-O-acetyl-D-galactonic acid with P(OEt)3 at <25° and heating 0.5 hr at 60° gave 90% syrupy di-Et 1-oxo-D-galacto-2,3,4,5,6-pentaacetoxyhexylphosphonate.
- IT 31022-55-6P 33579-60-1P
- RN 31022-55-6 CAPLUS
- CN Phosphonic acid, [D-glycero-D-gulo(or D-glycero-D-ido)-1,2,3,4,5,6-hexahydroxyhexyl]-, diphenyl ester, 2,3,4,5,6-pentaacetate (8CI) (CA INDEX NAME)

- RN 33579-60-1 CAPLUS
- CN Phosphonic acid, [D-glycero-L-gluco(or D-glycero-L-manno)-1,2,3,4,5,6-hexahydroxyhexyl]-, diethyl ester, 2,3,4,5,6-pentaacetate (8CI) (CA INDEX NAME)

- L7 ANSWER 55 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 1971:42579 CAPLUS <<LOGINID::20080519>>
- DN 74:42579
- OREF 74:6861a,6864a
- TI Carbon-phosphorus bond in carbohydrates
- AU Zhdanov, Yu. A.; Uzlova, L. A.
- CS Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR
- SO Zhurnal Obshchei Khimii (1970), 40(9), 2138 CODEN: ZOKHA4; ISSN: 0044-460X
- DT Journal
- LA Russian
- AB The normal Arbuzov rearrangement of P(OR)3 performed with carbonyl forms of aldoses, chlorides of aldonic acids and tetra-O-acetylgalactaroyl

dichloride gave sugar phosphonic acids esters with C-P bonds. R'CH(OH)PO(OR)2 (R' = sugar residue) were stable on storage and were prepared from the aldehydo-forms of the sugars. R'C(O)PO(OR)2 were unstable on storage and were prepared from the chlorides of sugar acids. Di-Ph 2,3,4,5 -D - gluco-pentaacetoxy - 1 - hydroxyhexyl)phosphonate and the di-Et ester analog were prepared in 62 and 51.5% yields, resp. Also prepared in 48-92% yields were: di-Et (1-hydroxy-2,8:4,5-di-O-isopropylidene- L-arabinitol- 1 -yl)phosphonate, di-Et (1-oxo-2,3,4,5,6-D-gluco-pentaacetoxyhexyl)-phosphonate, di-Et (1-oxo-2,3,4,5,6-pentaacetoxy-D-galacto-hexyl)phosphonate, the di-iso-Pr ester analog, tetra-Et (1,6-dioxo-2,3,4,5,6-D-galacto-tetraacetoxyhexane)diphosphonate, and its tetra-iso-Pr ester analog.

IT 31022-52-3P 31022-53-4P 31022-54-5P

31022-55-6P

RN 31022-52-3 CAPLUS

CN Phosphonic acid, (D-glycero-D-ido-1,2,3,4,5,6-hexahydroxyhexyl)-, diethyl ester, 2,3,4,5,6-pentaacetate (8CI) (CA INDEX NAME)

RN 31022-53-4 CAPLUS

CN Phosphonic acid, (D-glycero-D-gulo-1,2,3,4,5,6-hexahydroxyhexyl)-, diethyl ester, 2,3,4,5,6-pentaacetate (8CI) (CA INDEX NAME)

RN 31022-54-5 CAPLUS

CN Phosphonic acid, (D-glycero-D-ido-1,2,3,4,5,6-hexahydroxyhexyl)-, diphenyl ester, 2,3,4,5,6-pentaacetate (8CI) (CA INDEX NAME)

RN 31022-55-6 CAPLUS

CN Phosphonic acid, [D-glycero-D-gulo(or D-glycero-D-ido)-1,2,3,4,5,6-hexahydroxyhexyl]-, diphenyl ester, 2,3,4,5,6-pentaacetate (8CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 56 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN L7

1970:100882 CAPLUS <<LOGINID::20080519>> ΑN

DN 72:100882

OREF 72:18317a,18320a

(1,2-Epoxypropyl)phosphonic acids, esters, and salts ΤI

Pollak, Peter I.; Christensen, Burton G.; Wendler, Norman L. IN

PΑ Merck and Co., Inc.

SO Ger. Offen., 84 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.	CNT 1				
	PATENT NO.	KIND 	DATE	APPLICATION NO.	DATE
ΡI	DE 1924169	 A	19700205		19690512
	DE 1924169	В2	19730705		
	DE 1924169	С3	19740221		
	US 3649619	A	19720314	US 1968-729424	19680515
	US 3652739	A	19720328	US 1968-755729	19680827
	CH 529795	A	19721031	СН 1968-529795	19681021
	BE 723078	A	19690429	BE 1968-723078	19681029
	BR 6803536	D0	19730222	BR 1968-203536	
	GB 1266611	A	19720315	GB 1969-1266611	19690512
	CA 939366	A1	19740101	CA 1969-51319	19690512
	BE 733050	A	19691114	BE 1969-733050	19690514
	NL 6907465	A	19691118	NL 1969-7465	19690514
	CH 513924	A	19711015	CH 1969-513924	19690514
	ES 367269	A1	19720216	ES 1969-367269	19690514
	AT 306052	В	19730326	AT 1969-4628	19690514
	FI 53216	В	19771130	FI 1969-1443	
	HU 164285	В	19740128	HU 1969-ME1074	19690515
	JP 49019264	В	19740516	JP 1969-37097	19690515
	CS 157064	В2	19740823	CS 1969-3446	19690515
	PL 81201	B1	19750830	PL 1969-133597	19690515
	FR 2008620	A5	19700123	FR 1969-15925	19690516
	FR 2008620	B1	19751031		
	ES 395152	A1	19741116	ES 1971-395152	
	ES 395153	A1	19741116	ES 1971-395153	19710916
	ES 395155	A1	19741116	ES 1971-395155	
	ES 395161	A1	19741116	ES 1971-395161	
	US 3819676	А	19740625	US 1972-217264	19720112
PRAI	US 1968-729424	A			
	US 1968-755729	A	19680827		
	US 1969-819447	A	19690425		
7\ TD	$\lambda_{n+i}$ biotic $(+)$ - or	d (-)-a	$i_{c-1}$ 2-ones	nronanenhos-phonic :	bacid (I) and

AΒ Antibiotic  $(\pm)$  - and (-) -cis-1,2-epoxypropanephos-phonic acid (I) and numerous derivs. were prepared Di-Me threo-1-hydroxy-2chloropropanephosphonate, prepared from equimolar amts. of 2-chloropropionaldehyde and P(OMe)3, was titrated in MeOH with 1.08N NaOH and phenolphthalein to give cis-I di-Me ester, which on refluxing with Me3SiCl, extracting with H2O, and treating with NaOH gave cis-I di-Na salt. cis-I di-Et ester was prepared from 2-acetoxypropionaldehyde in C6H6 by reaction with P(OEt)3 to give di-Et threo-1-hydroxy-2acetoxypropanephosphonate, which was treated with MeSO2Cl to give the methylsulfonyloxy compound (II), which was cyclized. 2-Aminopropionaldehyde and P(OPr)3 gave di-Pr threo-1-hydroxy-2-aminopropanephosphonate, from which [1-[bis(propyloxy)phosphinyl]-1-hydroxy-2-propyl]trimethylammonium iodide and cis-I di-Pr ester were prepared cis-I di-Bu ester was prepared from 2-ethylthiopropionaldehyde and P(OBu)3 via di-Bu threo-1 -hydroxy - 2 -ethylthiopropanephosphonate and threo-[1 - [bis-(butyloxy)phosphinyl] - 1 - hydroxy - 2 - propyl] diethylsulfonium iodide. threo- 1 - Hydroxy - 2 trichloroacetoxypropanephosphonic acid was prepared from cis-1-propenephosphonic acid (III), BzOOH, and Cl3CCO2H and gave cis-I di-Na salt via II pyridine salt. Addnl. similar compds. were prepared Di-Me (1S,2S)-threo- 1 - hydroxy - 2 - trifluoroacetoxypropanephosphonate (from (+)-(1S,2R)-cis-I di-Me ester and CF3CO2H) gave via the methylsulfonyloxy compound (-)-(1R,2S)-cis-I di-Me ester,  $[\alpha]D$ 6.1° (MeOH). Similarly from (+)-cis-I via threo-1-hydroxy-2acetoxypropanephosphonic acid (-)-cis-I, m. 170° (decomposition),  $[\alpha]$  0405 -16° (c 3, H2O) was obtained. Other routes to I di-Me ester are described. (±)-threo-1-Chloro-2hydroxypropanephosphonic acid (IV), m.  $151-3^{\circ}$ , was obtained in 71.3% yield from 0.599 g III in 2 ml H2O and 0.585 ml tert-BuO-Cl at 0°; from IV (±)-cis-I Ca salt was prepared (+)-threo-IV, m.  $107-8^{\circ}$ , [ $\alpha$ ] 405 19.03° (c 3.415, H2O) was also prepared 26383-77-7P 26383-86-8P 26612-53-3P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 26383-77-7 CAPLUS

Phosphonic acid, (1,2-dihydroxypropyl)-, diethyl ester, 2-acetate, threo-

Relative stereochemistry.

(8CI) (CA INDEX NAME)

ΙT

RN CN

RN 26383-86-8 CAPLUS

CN Acetic acid, trichloro-, 2-ester with (1,2-dihydroxypropyl)phosphonic acid, threo- (8CI) (CA INDEX NAME)

Relative stereochemistry.

26612-53-3 CAPLUS RN

Acetic acid, trifluoro-, 2-ester with dimethyl (1,2-CN dihydroxypropyl)phosphonate, (1S,2S)-threo- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

T.7

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ANSWER 57 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
ΑN
     DN
     72:67049
OREF 72:12251a,12254a
     Synthesis and transformations in the phosphonomycin series
TI
     Girotra, Narindar N.; Wendler, N. L.
ΑU
    Merck Sharp and Dohme Res. Lab., Merck and Co., Inc., Rahway, NJ, USA
CS
SO
     Tetrahedron Letters (1969), (53), 4647-50
    CODEN: TELEAY; ISSN: 0040-4039
DT
     Journal
LA
    English
GΙ
     For diagram(s), see printed CA Issue.
     (cis-1-Propenyl)phosphonic acid (I) is treated with tert-BuOCl or Na OCl
AΒ
     to give 85% threo acid II, m. 152-4°. II is resolved with
     (-)-PhCHMeNH2 to give 80% (+)-chlorohydrin, m. 107.5-8.5°,
     [\alpha]\,405\,\,19.03\,^{\circ} (c 3.415, water), which is treated with 10N N
     aOH to give 85-90% (-)-phosphonomycin (III). III has the
     1R:2S-configuration. III is treated with CH2N2 to give IV, b2
     55-6^{\circ}, [\alpha] 578 6.11^{\circ} (c 4.335, MeOH); IV is treated
     with 48% aqueous HBr-CHCl3 to give three compound V, b0.2 123-5°,
     [\alpha]578 -30.12^{\circ} (c 4.35, CHCl3). The hydrogenolysis
     (Pd/CaCO3) of V in MeOH gives R-VI, b0.075 89-90°, [\alpha] 578
     -18.3° (c 4.58, MeOH). I and N-bromosuccinimide give VII, m.
     135-7^{\circ}; III is also prepared from VII. III (Na salt) is treated with
     HBr and HCl to give VIII, m. 150-2^{\circ}, and IX, m. 157-60^{\circ}.
     VIII and IX are treated with aqueous NaHCO3 and immediately rearrange to
     1-formyl ethanephosphonic acid; 2,4-dinitrophenylhydrazone m.
     198-200°. IV is converted to X (XI b0.1, 71-2°); and X is
     treated with MeSO2Cl-pyridine to give XII. XII is treated with OH- to
     give XIII, [\alpha]578 - 6.0^{\circ} (c 2.75, MeOH).
ΙT
     25449-90-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     25449-90-5 CAPLUS
RN
     Acetic acid, trifluoro-, 2-ester with dimethyl (1,2-
```

dihydroxypropyl)phosphonate, stereoisomer (8CI) (CA INDEX NAME)

L7 ANSWER 58 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1958:103886 CAPLUS <<LOGINID::20080519>>

DN 52:103886

OREF 52:18223d-e

TI New derivative from aldehydo-D-glucose pentaacetate. Dimethyl 2,3,4,5,6-D -glucopentaacetoxy-1-hydroxyhexylphosphonate

AU Alexander, B. H.; Barthel, W. F.

CS U.S. Dept. Agr., Beltsville, MD

SO Journal of Organic Chemistry (1958), 23, 101 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

AB cf. C.A. 50, 3207h. The title compound (I) proved to be of little value as an insecticide. Freshly distilled Me2HPO3 (0.02 mole) and 0.005 mole aldehydo-D-glucose pentaacetate (cf. Wolfrom, et al., C.A. 33, 33369) treated with 8 drops 1:2 NMe3-absolute alc. and the mixture shaken 30 sec. at 100°, kept at 5° several days, and the Et2O-washed crystals recrystd. (Me2CO or alc.) yielded 20% I, m. 172-3°, [ $\alpha$ ]D24 25° (c 2, CHCl3).

RN 112137-62-9 CAPLUS

CN Phosphonic acid, D-gluco-1,2,3,4,5,6-hexahydroxyhexyl-, dimethyl ester, 2,3,4,5,6-pentaacetate (6CI) (CA INDEX NAME)

Absolute stereochemistry.

=> d 17 1-49 bib abs hitstr THE ESTIMATED COST FOR THIS REQUEST IS 267.05 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L7 ANSWER 1 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2007:585890 CAPLUS <<LOGINID::20080519>>

DN 147:188986

TI  $\alpha$ -substituted phosphonate analogues of lysophosphatidic acid (LPA)

selectively inhibit production and action of LPA

- AU Jiang, Guowei; Xu, Yong; Fujiwara, Yuko; Tsukahara, Tamotsu; Tsukahara, Ryoko; Gajewiak, Joanna; Tigyi, Gabor; Prestwich, Glenn D.
- CS Department of Medicinal Chemistry, The University of Utah, Salt Lake City, UT, 84108-1257, USA
- SO ChemMedChem (2007), 2(5), 679-690 CODEN: CHEMGX; ISSN: 1860-7179
- PB Wiley-VCH Verlag GmbH & Co. KGaA
- DT Journal
- LA English
- AΒ Isoform-selective agonists and antagonists of the lysophosphatidic acid (LPA) G-protein-coupled receptors (GPCRs) have important potential applications in cell biol. and therapy. LPA GPCRs regulate cancer cell proliferation, invasion, angiogenesis, and biochem. resistance to chemotherapy- and radiotherapy-induced apoptosis. LPA and its analogs are also feedback inhibitors of the enzyme lysophospholipase D (lysoPLD, also known as autotaxin), a central regulator of invasion and metastasis. For cancer therapy, the ideal therapeutic profile would be a metabolically stabilized pan-LPA receptor antagonist that also inhibits lysoPLD. Herein we describe the synthesis of a series of novel  $\alpha$ -substituted methylene phosphonate analogs of LPA. Each of these analogs contains a hydrolysis-resistant phosphonate mimic of the labile monophosphate of natural LPA. The pharmacol. properties of these phosphono-LPA analogs were characterized in terms of LPA receptor subtype-specific agonist and antagonist activity using Ca2+ mobilization assays in RH7777 and CHO cells expressing the individual LPA GPCRs. In particular, the methylene phosphonate LPA analog is a selective LPA2 agonist, whereas the corresponding  $\alpha$ -hydroxymethylene phosphonate is a selective LPA3 agonist. Most importantly, the  $\alpha$ -bromomethylene and  $\alpha$ -chloromethylene phosphonates show pan-LPA receptor subtype antagonist activity. The  $\alpha$ -bromomethylene phosphonates are the first reported antagonists for the LPA4 GPCR. Each of the  $\alpha$ -substituted methylene phosphonates inhibits lysoPLD, with the unsubstituted methylene phosphonate showing the most potent inhibition. Finally, unlike many LPA analogs, none of these compds. activate the intracellular LPA receptor PPARy.
- IT 944265-54-7P 944265-56-9P 944265-66-1P 944265-68-3P 944265-85-4P 944265-86-5P 944265-87-6P 944265-88-7P 944265-98-9P 944265-99-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and LPA receptor subtype-specific agonist and antagonist activities of  $\alpha$ -substituted phosphonate analogs of lysophosphatidic acid (LPA))

RN 944265-54-7 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-2-hydroxy-4-phosphonobutyl ester, sodium salt (1:1) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Na

RN 944265-56-9 CAPLUS

CN Hexadecanoic acid, (2S)-2-hydroxy-4-phosphonobutyl ester, sodium salt (1:1) (CA INDEX NAME)

Absolute stereochemistry.

Na

RN 944265-66-1 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-2,4-dihydroxy-4-phosphonobutyl ester, sodium salt (1:1) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Na

RN 944265-68-3 CAPLUS

CN Hexadecanoic acid, (2S)-2, 4-dihydroxy-4-phosphonobutyl ester, sodium salt (1:1) (CA INDEX NAME)

Na

RN 944265-85-4 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-chloro-2-hydroxy-4-phosphonobutyl ester, sodium salt (1:1) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Na

RN 944265-86-5 CAPLUS

CN Hexadecanoic acid, (2S)-4-chloro-2-hydroxy-4-phosphonobutyl ester, sodium salt (1:1) (CA INDEX NAME)

Absolute stereochemistry.

● Na

RN 944265-87-6 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-bromo-2-hydroxy-4-phosphonobutyl ester, sodium salt (1:1) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Na

RN 944265-88-7 CAPLUS

CN Hexadecanoic acid, (2S)-4-bromo-2-hydroxy-4-phosphonobutyl ester, sodium salt (1:1) (CA INDEX NAME)

Absolute stereochemistry.

Na

RN 944265-98-9 CAPLUS

CN Hexadecanoic acid, (2S, 4S)-2, 4-dihydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 944265-99-0 CAPLUS

CN Hexadecanoic acid, (2S, 4R)-2, 4-dihydroxy-4-phosphonobutyl ester (CA INDEX NAME)

IT 944265-50-3P 944265-52-5P 944265-62-7P

944265-64-9P 944265-79-6P 944265-81-0P

944265-83-2P 944265-84-3P 944265-96-7P

944265-97-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and LPA receptor subtype-specific agonist and antagonist activities of  $\alpha\text{-substituted}$  phosphonate analogs of

lysophosphatidic acid (LPA))

RN 944265-50-3 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-(diethoxyphosphinyl)-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 7 
$$\underline{Z}$$
 (CH<sub>2</sub>) 7  $0$  S  $P$   $0$  EtO

RN 944265-52-5 CAPLUS

CN Hexadecanoic acid, (2S)-4-(diethoxyphosphinyl)-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 944265-62-7 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-(dimethoxyphosphinyl)-2,4-dihydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me 
$$(CH_2)$$
 7  $Z$   $(CH_2)$  7  $O$   $S$   $OH$   $OH$   $OH$   $OMe$   $OMe$ 

RN 944265-64-9 CAPLUS

CN Hexadecanoic acid, (2S)-4-(dimethoxyphosphinyl)-2,4-dihydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 944265-79-6 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-chloro-4-(diethoxyphosphinyl)-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Me (CH<sub>2</sub>) 7 
$$\underline{z}$$
 (CH<sub>2</sub>) 7  $\underbrace{CH_2}_{O}$  0  $\underbrace{CH_2}_{O}$  0

RN 944265-81-0 CAPLUS

CN Hexadecanoic acid, (2S)-4-chloro-4-(diethoxyphosphinyl)-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 944265-83-2 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-bromo-4-(diethoxyphosphinyl)-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Me (CH<sub>2</sub>) 7 
$$\underline{Z}$$
 (CH<sub>2</sub>) 7  $\underline{O}$  S  $\underbrace{CH_{2}}_{O}$  OEt  $\underbrace{CH_{2}}_{O}$  O  $\underbrace{CH_{2}}_{O}$  OET

RN 944265-84-3 CAPLUS

CN Hexadecanoic acid, (2S)-4-bromo-4-(diethoxyphosphinyl)-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 944265-96-7 CAPLUS

CN Hexadecanoic acid, (2S, 4S)-4-(dimethoxyphosphinyl)-2, 4-dihydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 944265-97-8 CAPLUS

CN Hexadecanoic acid, (2S,4R)-4-(dimethoxyphosphinyl)-2,4-dihydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RE.CNT 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 2 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2007:499046 CAPLUS <<LOGINID::20080519>>
- DN 147:160383
- TI Linoleoyl lysophosphatidic acid and linoleoyl lysophosphatidylcholine are efficient substrates for mammalian lipoxygenases
- AU Huang, Long Shuang; Kim, Mee Ree; Jeong, Tae-Sook; Sok, Dai-Eun
- CS College of Pharmacy, Chungnam National University, Taejon, S. Korea
- SO Biochimica et Biophysica Acta, General Subjects (2007), 1770(7), 1062-1070 CODEN: BBGSB3; ISSN: 0304-4165
- PB Elsevier Ltd.
- DT Journal
- LA English
- AB Oxygenation of two lysophospholipids, 1-linoleoyl lysophosphatidylcholine (linoleoyl-lysoPC) and 1-linoleoyl lysophosphatidic acid (linoleoyl-lysoPA), by reticulocyte lipoxygenase (LOX) or porcine leukocyte LOX was measured by monitoring the formation of conjugated

dienes. Consistent with the above, the formation of linoleoyllysophospholipid hydroperoxide as oxygenation product was confirmed by LC/MS analyses. In further study, the oxygenation products of linoleoyl-lysoPC or linoleoyl-lysoPA were found to contain hydroperoxide group predominantly at C-13 with the S enantiomer as a major one, in a good agreement with the positional-specificity and stereo-selectivity of reticulocyte LOX or leukocyte LOX in oxygenation of linoleic acid. The kinetic study indicates that linoleoyl-lysoPA and linoleoyl-lysoPC are no less efficient than linoleic acid as substrates of reticulocyte LOX as well as leukocyte LOX. In contrast, these lysophospholipids were not oxygenated efficiently by potato LOX. Thus, linoleoyl-lysophospholipids such as linoleoyl-lysoPA or linoleoyl-lysoPC could be utilized as efficient substrates for some mammalian lipoxygenases.

IT 943836-74-6

RL: BSU (Biological study, unclassified); BIOL (Biological study) (linoleoyl lysophosphatidic acid and linoleoyl lysophosphatidylcholine are efficient substrates for mammalian lipoxygenases)

RN 943836-74-6 CAPLUS

CN 9,12-Octadecadienoic acid (9Z,12Z)-, 2-hydroxy-3-phosphonopropyl ester (CA INDEX NAME)

Double bond geometry as shown.

# RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 3 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2007:385493 CAPLUS <<LOGINID::20080519>>
- DN 146:381937
- TI Aqueous dispersion comprising at least 1 vinylidene chloride polymer and at least 1 copolymer having phosphonate groups for coatings
- IN Fringant, Christophe; Vanderveken, Yves; Loubat, Cedric; Boutevin, Gilles
- PA Solvay et Cie., Belg.
- SO Fr. Demande, 35pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

PAN.	7I/I T	Τ																
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DT	FR 2891548					7.1	_	2007	0.406					20051005				
ΡI	РK	Z891:	548			A1		20070406			FR 2	005-		20051005				
	WO	20070	0396:	26		A1 20070412				•	WO 2	006-		20061004				
		W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
			GE,	GH,	GM,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KN,	KP,
			KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,
			MW,	MX,	MY,	MΖ,	NA,	NG,	NI,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RS,
			RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,
			UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW							
		RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,
			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
			CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI FR 2005-10182 A 20051005

AB Aqueous dispersion vinylidene chloride polymer coatings with improved adhesion to metals and plastics contain  $\geq 1$  copolymer (I) containing repeating units having  $\geq 1$  PO(OH)(OR1) (R1 = H or C1-11 alkyl) and repeating units derived from monomers selected from styrene, maleic anhydride, itaconic acid and CH2:CR2R3 [R2 = H or Me; R3 = CN or COR4; R4 = OH, OR5, or NR6R7; R5 = C1-18 alkyl optionally substituted by  $\geq 1$  OH, epoxy-C2-10-alkyl, or alkoxy-C2-10-alkyl; R6, R7 = H or ( $\geq 1$  OH-containing) C1-10 alkyl]. A typical I was manufactured by radical emulsion polymerization of 22 g Me methacrylate (II) and 1 g CH2:CMeCO2CH2P(:O)(OH)(OMe) in the presence of an emulsion prepared by radical polymerization of 2 g II in

the

presence of 0.625 g polystyrene seeds.

IT 932019-49-3P

RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (aqueous dispersions containing vinylidene chloride polymers and copolymers having phosphonate groups for coatings for metals and plastics)

RN 932019-49-3 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 2-hydroxy-2-phosphonopropyl ester, polymer with methyl 2-methyl-2-propenoate (CA INDEX NAME)

CM 1

CRN 932019-48-2 CMF C7 H13 O6 P

CM 2

CRN 80-62-6 CMF C5 H8 O2

## RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2007:330986 CAPLUS <<LOGINID::20080519>>

DN 146:501119

TI Convenient and regioselective one-pot solvent-free synthesis of  $\beta\text{-hydroxyphosphonates}$ 

AU Sardarian, A. R.; Shahsavari-Fard, Z.

CS Chemistry Department, College of Science, Shiraz University, Shiraz, Iran

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SO Synthetic Communications (2007), 37(2), 289-295 CODEN: SYNCAV; ISSN: 0039-7911
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- PB Taylor & Francis, Inc.
- DT Journal
- LA English
- OS CASREACT 146:501119
- AB A simple, efficient, regioselective, and solvent-free method has been developed for the synthesis of  $\beta$ -hydroxyphosphonates from epoxides and tri-Et phosphite using ZnCl2 in high yields under mild conditions.
- IT 639470-55-6P
  - RL: SPN (Synthetic preparation); PREP (Preparation) (regionselective phosphorylation of epoxides using a one-pot solvent-free method for the synthesis of  $\beta$ -hydroxyphosphonates)
- RN 639470-55-6 CAPLUS
- CN 2-Propenoic acid, 2-methyl-, 3-(diethoxyphosphinyl)-2-hydroxypropyl ester (CA INDEX NAME)

## RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 5 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2005:1321914 CAPLUS <<LOGINID::20080519>>
- DN 145:167332
- TI Studies on organophosphorus compounds 135. A facile chemoenzymatic method for the preparation of chiral 1,2-dihydroxy-3,3,3-trifluoropropanephosphonates
- AU Yuan, Chengye; Li, Jinfeng; Zhang, Wenchi
- CS State Key Laboratory of Bio-organic and Natural Products Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 354 Feng-Lin Lu, Shanghai, 200032, Peop. Rep. China
- SO Journal of Fluorine Chemistry (2006), 127(1), 44-47 CODEN: JFLCAR; ISSN: 0022-1139
- PB Elsevier B.V.
- DT Journal
- LA English
- OS CASREACT 145:167332
- AB A convenient and effective method for the preparation of chiral di-Et 3,3,3-trifluoro-1,2-dihydroxypropylphosphonates based on a chemoenzymic approach is described. Et trifluoroacetate was reacted with anion of di-Et methylphosphonate to give di-Et 2-oxo-3,3,3-trifluoropropylphosphonate and its hydrates, di-Et 2,2-dihydroxy-3,3,3-trifluoropropylphosphonates, which were reduced with NaBH4 affording di-Et 2-hydroxy-3,3,3-trifluoropropylphosphonates. The product thus obtained was then converted to corresponding di-Et 3,3,3-trifluoroprop-1-enylphosphonate and followed by diastereoselective 1,2-dihydroxylation via KMnO4 treatment. Enzymic kinetic resolution of the 0,0-diacyl racemate CF3CH(O2CCH2Cl)CH(O2CCH2Cl)P(O)(OEt)2 by CALB (Novozym 345) or M. miehei lipase (Lipozyme IM) provided (after further chemical hydrolysis) optically active di-Et 1,2-dihydroxy-3,3,3-trifluoropropylphosphonate with satisfactory chemical and enantiomeric yield.
- IT 900523-58-2P, Diethyl [(1R,2R)-1-(chloroacetoxy)-3,3,3-trifluoro-2-hydroxypropyl]phosphonate

RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(hydrolysis; facial chemoenzymic method for preparation of chiral di-Et 1,2-dihydroxy-3,3,3-trifluoropropylphosphonates)

RN 900523-58-2 CAPLUS

CN Acetic acid, 2-chloro-, (1R,2R)-1-(diethoxyphosphinyl)-3,3,3-trifluoro-2-hydroxypropyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

### RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:1241343 CAPLUS <<LOGINID::20080519>>

DN 144:129169

TI Enantiomerically pure 4-amino-1,2,3-trihydroxybutylphosphonic acids

AU Wroblewski, Andrzej E.; Glowacka, Iwona E.

CS Bioorganic Chemistry Laboratory, Faculty of Pharmacy, Medical University of Lodz, Lodz, 90-151, Pol.

SO Tetrahedron (2005), 61(50), 11930-11938 CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier B.V.

DT Journal

LA English

OS CASREACT 144:129169

AB (1S,2R,3S)-, (1R,2R,3S)- and (1S,2R,3R)-4-amino-1,2,3-trihydroxybutylphosphonic acids were synthesized. The synthetic strategy involved preparation of the resp. 4-azido-2,3-0-isopropylidene-L-threose or -D-erythrose, addition of dialkyl phosphites, separation of C-1 epimeric O,0-dibenzyl phosphonates, the reduction of azides and the removal of the protecting groups. The (2R,3S) and (2R,3R) configurations in the final products were secured by employing di-Et L-tartrate and D-isoascorbic acid as starting materials. The stereochem. course of the addition to the carbonyl groups in 4-azido-2,3-0-isopropylidene-L-threose or -D-erythrose followed that established earlier for 2,3-0-isopropylidene-D-glyceraldehyde and similar (3:1)-(4:1) diastereoselectivities were achieved.

IT 873550-88-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (diastereoselective preparation of (1S,2R,3S)-, (1R,2R,3S)- and (1S,2R,3R)-4-amino-1,2,3-trihydroxybutylphosphonic acids)

RN 873550-88-0 CAPLUS

CN Phosphonic acid, [(1S,2R,3S)-2,3-bis(acetyloxy)-4-azido-1-hydroxybutyl]-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

### RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

ΑN

143:347057 DN

TΙ Preparation of piperidinecarboxylate derivatives for the treatment of migraine

ΙN Degnan, Andrew P.; Han, Xiaojun; Dubowchik, Gene M.; Macor, John E.; Mercer, Stephen E.

PAUSA

SO U.S. Pat. Appl. Publ., 76 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.					KIND DATE								DATE					
PI	US 20 AU 20 CA 25	US 20050215576 UJ 2005228881 UA 2562039 UJ 2005095383					2005 2005 2005		US 2 AU 2 CA 2	005- 005- 005-	9142 2288 2562	9 81 039		20050328				
	И	V: AE, CN, GE, LK, NO, SY, RW: BW, AZ, EE,	AG, CO, GH, LR, NZ, TJ, GH, BY,	AL, CR, GM, LS, OM, TM, GM, KG, FI,	AM, CU, HR, LT, PG, TN, KE, KZ, FR, SK,	AT, CZ, HU, LU, PH, TR, LS, MD, GB,	AU, DE, ID, LV, PL, TT,	AZ, DK, IL, MA, PT, TZ, MZ, TJ, HU,	BA, DM, IN, MD, RO, UA, NA, TM, IE,	BB, DZ, IS, MG, RU, UG, SD, AT, IS,	BG, EC, JP, MK, SC, US, SL, BE, IT,	BR, EE, KE, MN, SD, UZ, SZ, BG, LT,	BW, EG, KG, MW, SE, VC, TZ, CH, LU,	BY, ES, KP, MX, SG, VN, UG, CY, MC,	BZ, FI, KR, MZ, SK, YU, ZM, CZ, NL,	CA, GB, KZ, NA, SL, ZA, ZW, DE,	CH, GD, LC, NI, SM, ZM, AM, DK, PT,	ZW
		730137 R: AT, IS,	BE,	BG, LI,	A1 CH,	CY,		DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	
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OS	CASRE	CACT 14	3:34	7057	; MA:	RPA]	: 143	:34/	057									

CASREACT 143:347057; MARPAT 143:347057

GΙ

AB Compds. of formula I [V = (substituted) NH2, alkoxy, phenoxy, (substituted) piperidinyl, piperazinyl, etc.; Q = heterocyclylmethyl, etc.; D = O, NCN, NSO2-alkyl; A = C, N, CH, COH; X = (CH2)m; Y = (CH2)n; m, n = 0-2; R = (substituted) oxoquinazolinyl, isoquinolinyl, etc.] are prepared as antagonists of calcitonin gene-related peptide receptors. The compds. can be used for the treatment of neurogenic vasodilation, neurogenic inflammation, migraine and other headaches, thermal injury, circulatory shock, flushing associated with menopause, airway inflammatory diseases, such as asthma and chronic obstructive pulmonary disease (COPD), and other conditions the treatment of which can be effected by the antagonism of CGRP-receptors. Thus, II was prepared The prepared compds. had binding affinities of less than 1 nM against human CGRP receptor.

(preparation of piperidinecarboxylate derivs. for treatment of migraine)

RN 205264-44-4 CAPLUS

CN Acetic acid, (acetyloxy)(diethoxyphosphinyl) - (9CI) (CA INDEX NAME)

- L7 ANSWER 8 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2005:547602 CAPLUS <<LOGINID::20080519>>
- DN 143:78091
- TI Preparation of heterocycles, particularly piperazines, as calcitonin gene-related peptide receptor antagonists and antimigraine agents
- IN Luo, Guanglin; Chen, Ling; Degnan, Andrew P.; Dubowchik, Gene M.; Macor, John E.; Tora, George O.; Chaturvedula, Prasad V.
- PA Bristol-Myers Squibb Company, USA
- SO PCT Int. Appl., 227 pp. CODEN: PIXXD2
- DT Patent

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ΡI		2005				A2 20050623					WO	2004-		20041206				
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		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB	, BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DΖ	, EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	IS	, JP,	KE,	KG,	KP,	KR,	KΖ,	LC,
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	JΡ	2007	5169					2007	0628			2006-					0041	206
	ΙN	2006	DN02					2007	0810		IN	2006-	DN27	41		2	0060	516
	MX	2006	PA05	970		Α		2006	0706		MX	2006-	PA59	70		2	0060	525
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CASREACT 143:78091; MARPAT 143:78091

WO 2004-US40721

OS

GI

ring; q = 0-1; V' = (un)substituted cycloalkyl, Ph, adamantyl, pyrrolyl, pyridazinyl, etc.; U = CH2, O, NH; Q = BR3, R3; B = alkylene, alkylydene; R3 = 4-6 membered heterocycle, cycloalkyl, Ph, naphthyl, etc., with proviso; A = C, N, NH; m, n = independently 0-2; provided that if <math>m, n = independently 00; then A is not N; if m = 2, then n is not 2; or if n is 2, then m is not 2; E = N, CH, C; p = 0-1; if p = 1, then GJE = (un) substituted fused heterocycle, 4-6-membered heterocycle; if p = 0, then A = C; GJA =spirocyclic ring with said rings of said system containing A and wherein GJA = (un) substituted fused heterocycle, 4-6-membered heterocycle; and their pharmaceutically acceptable salts and solvates] were prepared as antagonists of calcitonin gene-related peptide (CGRP) receptors, especially CGRP type 1 (CGRP1) receptors for treating migraines. For example, reaction of 4-(7-Methyl-1H-indazol-5-yl)-3-(pyridin-2-yl)butanoic acid (preparation given) with 3-(Piperidin-4-yl)-3,4-dihydroquinazolin-2(1H)-one gave II. Selected I bound to human CGRP1 receptor with IC50 values < 10 nM. I and their pharmaceutical compns. are useful in the treatment of neurogenic vasodilation, neurogenic inflammation, migraine and other headaches, thermal injury, circulatory shock, flushing associated with menopause, airway inflammatory diseases, such as asthma and chronic obstructive pulmonary disease (COPD), and other conditions the treatment of which can be effected by the antagonism of CGRP-receptors.

IT 205264-44-4P, 2-Acetoxy-2-(diethoxyphosphoryl)acetic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(intermediate; preparation of heterocycles, particularly piperazines, as calcitonin gene-related peptide receptor antagonists and antimigraine agents)

RN 205264-44-4 CAPLUS

CN Acetic acid, (acetyloxy) (diethoxyphosphinyl) - (9CI) (CA INDEX NAME)

- L7 ANSWER 9 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2005:286164 CAPLUS <<LOGINID::20080519>>
- DN 142:456268
- TI Structure-Activity Relationships of Fluorinated Lysophosphatidic Acid Analogues
- AU Xu, Yong; Aoki, Junken; Shimizu, Kumiko; Umezu-Goto, Makiko; Hama, Kotaro; Takanezawa, Yasukazu; Yu, Shuangxing; Mills, Gordon B.; Arai, Hiroyuki; Qian, Lian; Prestwich, Glenn D.
- CS Department of Medicinal Chemistry and The Center for Cell Signaling, University of Utah, Salt Lake City, UT, 84108-1257, USA
- SO Journal of Medicinal Chemistry (2005), 48(9), 3319-3327 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- LA English
- AB Lysophosphatidic acid (LPA, 1- or 2-acyl-sn-glycerol 3-phosphate) displays an intriguing cell biol. that is mediated via interactions with seven-transmembrane G-protein-coupled receptors (GPCRs) and the nuclear hormone receptor PPAR $\gamma$ . To identify receptor-selective LPA analogs, we describe a series of fluorinated LPA analogs in which either the sn-1 or sn-2 hydroxyl group was replaced by a fluoro or fluoromethyl

substituent. We also describe stabilized phosphonate analogs in which the bridging oxygen of the monophosphate was replaced by an  $\alpha\text{-monofluoromethylene}$  (-CHF-) or  $\alpha\text{-difluoromethylene}$  (-CF2-) moiety. The sn-2- and sn-1-fluoro-LPA analogs were unable to undergo acyl migration, effectively "freezing" them in the sn-1-0-acyl or sn-2-0-acyl forms, resp. We first tested these LPA analogs on insect Sf9 cells induced to express human LPA1, LPA2, and LPA3 receptors. While none of the analogs were found to be more potent than 1-oleoyl-LPA at LPA1 and LPA2, several LPA analogs were potent LPA3-selective agonists. In contrast, 1-oleoyl-LPA had similar activity at all three receptors. The  $\alpha\text{-fluoromethylene}$  phosphonate analog activated calcium release in LPA3-transfected insect Sf9 cells at a concentration 100-fold lower than that

of

1-oleoyl-LPA. This activation was enantioselective, with the (2S)-enantiomer showing 1000-fold more activity than the (2R)-enantiomer. Similar results were found for calcium release in HT-29 and OVCAR8 cells.  $\alpha\text{-Fluoromethylene}$  phosphonate analog was also more effective than 1-oleoyl-LPA in activating MAPK and AKT in cells expressing high levels of LPA3. The  $\alpha\text{-fluoromethylene}$  phosphonate moiety greatly increased the half-life of  $\alpha\text{-fluoromethylene}$  phosphonate analog in cell culture. Thus,  $\alpha\text{-fluoromethylene}$  LPA analogs are unique new phosphatase-resistant ligands that provide enantiospecific and receptor-specific biol. readouts.

IT 565438-23-5 565438-27-9 565453-76-1 565453-77-2 748127-70-0 792182-75-3

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(structure-activity relationships of fluorinated lysophosphatidic acid analogs and LPA receptor-specific binding)

RN 565438-23-5 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 565438-27-9 CAPLUS

CN Hexadecanoic acid, (2S)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 565453-76-1 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2R)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 565453-77-2 CAPLUS

CN Hexadecanoic acid, (2R)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 748127-70-0 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2R)-4, 4-difluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 792182-75-3 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4,4-difluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

### RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:182218 CAPLUS <<LOGINID::20080519>>

DN 142:287808

TI Lithographic printing plate precursor for direct imaging from a digital data and developing in a printing machine without passing through a development step

IN Yamasaki, Sumiaki; Makino, Naonori; Inno, Toshifumi

PA Fuji Photo Film Co., Ltd., Japan

SO U.S. Pat. Appl. Publ., 50 pp. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

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	PAT	CENT	NO.			KIN:	D	DATE		Ā	APPL:	ICAT	DATE						
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PRAI	JΡ	2003	-277	448		A		2003	0722										
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	JΡ	P 2004-17599				Α	A 20040126												
	JP 2004-214190					Α	A 20040722												
OS	MAF	RPAT	142:2	2878	8 0														

AB A lithog. printing plate precursor is described for recording an image directly from a digital data and development in a printing machine without passing through a development step. The precursor provides lithog. printing plates with improved press life and stain resistance. Thus, the precursor coating composition comprises an image-forming layer containing a polymerization

initiator and a polymerizable compound, and a hydrophilic support. The composition includes a compound containing at least one functional group interacting

with a surface of the hydrophilic support . This compound is one of a phosphonic acid and a phosphoric acid amide.

IT 847204-76-6

RL: TEM (Technical or engineered material use); USES (Uses) (phosphonic derivative; lithog. printing plate precursor for direct imaging from digital data and in-press development)

RN 847204-76-6 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 2-hydroxy-3-phosphonopropyl ester (CA INDEX NAME)

### RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 11 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

- AN 2005:132714 CAPLUS <<LOGINID::20080519>>
- DN 142:355333
- TI Improved synthesis of 1,3-propanediol derivatives having a diethoxyphosphoryldifluoroethyl functional group at the 2-position: application to chemoenzymatic synthesis of novel acyclic nucleotide analogues of adenosine bisphosphates
- AU Murano, Tetsuo; Kobayakawa, Hirokuni; Yuasa, Yoko; Yokomatsu, Tsutomu; Shibuya, Shiroshi
- CS School of Pharmacy, Tokyo University of Pharmacy and Life Science, Tokyo, 192-0392, Japan
- SO Synthesis (2005), (2), 187-192 CODEN: SYNTBF; ISSN: 0039-7881
- PB Georg Thieme Verlag
- DT Journal
- LA English
- OS CASREACT 142:355333
- AB An alternative synthesis of di-Et 1,1-difluoro-4-hydroxy-3- (hydroxymethyl)butylphosphonate (1) having a diethoxyphosphoryldifluoroeth yl group was examined The method readily provided a multi-gram quantity of 1. Propanediol 1 was chemo-enzymically transformed to acyclic nucleotide analogs for adenosine bisphosphates.
- IT 182691-05-0P

RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of propanediol derivs. having a diethoxyphosphoryldifluoroethyl functional group for chemoenzymic synthesis of acyclic nucleotide analogs of adenosine bisphosphates)

- RN 182691-05-0 CAPLUS
- CN Phosphonic acid, [(3R)-4-(acetyloxy)-1,1-difluoro-3-(hydroxymethyl)butyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

### RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 12 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2003:882219 CAPLUS <<LOGINID::20080519>>
- DN 140:60042
- TI New phosphonated methacrylates: Synthesis, photocuring and study of their thermal and flame-retardant properties
- AU Youssef, Boulos; Lecamp, Laurence; El Khatib, Wassef; Bunel, Claude; Mortaigne, Bruno
- CS UMR 6522, Polymeres Biopolymeres Membranes, Laboratoire de Materiaux Macromoleculaires, Institut National des Sciences Appliquees de Rouen, Mont Saint Aignan, 76131, Fr.
- SO Macromolecular Chemistry and Physics (2003), 204(15), 1842-1850 CODEN: MCHPES; ISSN: 1022-1352
- PB Wiley-VCH Verlag GmbH & Co. KGaA
- DT Journal
- LA English

In this work, a new methacrylate phosphonate monomer synthesis was AΒ described according to two routes:. Firstly, by condensation of methacrylic acid with a phosphonate epoxide and. Secondly by an esterification between methacryloyl chloride and a phosphonate diol. The photoinduced polymerization of this new monomer was studied as a function of reaction temperature The optimal conversion of the photopolymn. was 81% for temps. below 60°C. Above 60°C, the existence of a thermal polymerization leads to a decrease in the apparent photochem. yield. monomer is less reactive than the com. dimethacrylate polyether of Bisphenol A we have used for copolymn. Mech. and thermal properties of the final copolymers were studied as a function of methacrylate phosphonate monomer content. Tg of the copolymers reaches a maximum when the phosphorus content is about 2%. The addition of phosphorus leads to an improvement of the thermal and flame-retardant properties. Thus, addition of 2% phosphorus allows us to decrease the degradation rate, to increase the amount.

of remaining residue after combustion up to 12%, and finally to increase the Limiting Oxygen Index (LOI) from 16.8 (0% P) to 21.4 (2% P).

IT 639470-55-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(monomer; synthesis and photocuring and study of thermal and flame-retardant properties of phosphonated methacrylate polymers)

RN 639470-55-6 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 3-(diethoxyphosphinyl)-2-hydroxypropyl ester (CA INDEX NAME)

$$^{\rm H_2C}$$
 O OH O  $_{\rm ||}$  || || Me-C-C-O-CH\_2-CH-CH\_2-P-OEt  $_{\rm ||}$  OEt

IT 639470-56-7P 639470-57-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and photocuring and study of thermal and flame-retardant properties of phosphonated methacrylate polymers)

RN 639470-56-7 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 3-(diethoxyphosphinyl)-2-hydroxypropyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 639470-55-6 CMF C11 H21 O6 P

RN 639470-57-8 CAPLUS

CN 2-Propenoic acid, 2-methyl-, 3-(diethoxyphosphinyl)-2-hydroxypropyl ester, polymer with  $\alpha, \alpha'$ -[(1-methylethylidene)di-4,1-

phenylene]bis[ $\omega$ -[(2-methyl-1-oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl)] (9CI) (CA INDEX NAME)

CM 1

CRN 639470-55-6 CMF C11 H21 O6 P

CM 2

CRN 41637-38-1

CMF (C2 H4 O)n (C2 H4 O)n C23 H24 O4

CCI PMS

PAGE 1-B

## RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 13 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2003:421543 CAPLUS <<LOGINID::20080519>>
- DN 139:133770
- TI Synthesis of  $\alpha$ -Fluorinated Phosphonates from  $\alpha$ -Fluorovinylphosphonates: A New Route to Analogues of Lysophosphatidic Acid
- AU Xu, Yong; Qian, Lian; Prestwich, Glenn D.
- CS Department of Medicinal Chemistry, University of Utah, Salt Lake City, UT, 84108-1257, USA
- SO Organic Letters (2003), 5(13), 2267-2270 CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREACT 139:133770

AB A versatile, efficient method for the preparation of  $\alpha$ -monofluoromethylene (-CHF-) phosphonates from  $\alpha$ -fluorovinylphosphonate provides access to a class of lysophosphatidic acid (LPA) receptor-subtype agonists. In addition, sn-2 O-methylation of  $\alpha$ -monofluoromethylene phosphonates using trimethylsilyldiazomethane generated sn-1-acyl, 2-O-Me  $\alpha$ -monofluoromethylene derivs. Finally, a novel method for the selective etherification of 1,2-diols was developed and a new class of sn-1 O-Me, 2-acyl  $\alpha$ -monofluoromethylene LPA analogs was prepared

IT 565438-17-7P 565438-19-9P 565438-21-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of  $\alpha$ -fluorinated phosphonates via O-methylation of  $\alpha$ -fluorovinylphosphonates as a route toward lysophosphatidic acid analogs)

RN 565438-17-7 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-(diethoxyphosphinyl)-4-fluoro-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Me (CH<sub>2</sub>) 7 
$$\underline{Z}$$
 (CH<sub>2</sub>) 7  $\underline{O}$  O  $\underline{S}$  P  $\underline{O}$  EtO

RN 565438-19-9 CAPLUS

CN 9,12-Octadecadienoic acid (9Z,12Z)-, (2S)-4-(diethoxyphosphinyl)-4-fluoro-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

Me (CH<sub>2</sub>)<sub>4</sub> 
$$\underline{z}$$
  $\underline{z}$  (CH<sub>2</sub>)<sub>7</sub>  $\underbrace{z}$  OEt

RN 565438-21-3 CAPLUS

CN Hexadecanoic acid, (2S)-4-(diethoxyphosphinyl)-4-fluoro-2-hydroxybutyl ester (CA INDEX NAME)

IT 565438-23-5P 565438-25-7P 565438-27-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of  $\alpha$ -fluorinated phosphonates via 0-methylation of  $\alpha$ -fluorovinylphosphonates as a route toward lysophosphatidic acid analogs)

RN 565438-23-5 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 565438-25-7 CAPLUS

CN 9,12-Octadecadienoic acid (9Z,12Z)-, (2S)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 565438-27-9 CAPLUS

CN Hexadecanoic acid, (2S)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

#### RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- ANSWER 14 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN L7
- ΑN
- 139:133754 DN
- TISynthesis of Monofluorinated Analogues of Lysophosphatidic Acid
- ΑU Xu, Yong; Qian, Lian; Prestwich, Glenn D.
- CS Department of Medicinal Chemistry and The Center for Cell Signaling, University of Utah, Salt Lake City, UT, 84108-1257, USA
- SO Journal of Organic Chemistry (2003), 68(13), 5320-5330 CODEN: JOCEAH; ISSN: 0022-3263
- PΒ American Chemical Society
- DT Journal
- LA English
- OS CASREACT 139:133754
- AΒ Lysophosphatidic acid (LPA, 1- or 2-acyl-sn-glycerol 3-phosphate) displays an intriguing cell biol. that is mediated via interactions both with G-protein coupled seven transmembrane receptors and with the nuclear hormone receptor PPAR $\gamma$ . Synthesis and biol. activities of fluorinated analogs of LPA are still relatively unknown. In an effort to identify receptor-selective LPA analogs and to document in detail the structure-activity relationships of fluorinated LPA isosteres, we describe a series of monofluorinated LPA analogs in which either the sn-1 or the sn-2 hydroxy group was replaced by fluorine, or the bridging oxygen in the monophosphate was replaced by an  $\alpha$ -monofluoromethylene (-CHF-) The sn-1 or sn-2 monofluorinated LPA analogs were enantiospecifically prepared from chiral protected glycerol synthons, and the lpha-monofluoromethylene-substituted LPA analogs were prepared from a racemic epoxide with use of a hydrolytic kinetic resolution The sn-2 and sn-1 fluoro LPA analogs were unable to undergo acyl migration, effectively "freezing" them in the sn-1-0-acyl or sn-2-0-acyl forms, resp. The  $\alpha$ -monofluoromethylene LPA analogs were unique new nonhydrolyzable ligands with surprising enantiospecific and receptor-specific biol. readouts, with one compound showing a 1000-fold higher activity than native LPA for one receptor subtype.
- 565438-17-7P 565438-21-3P 565453-74-9P ΙT

565453-75-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and platelet aggregation activation of monofluorinated and  $\alpha$ -fluoromethylene phosphonate analogs of lysophosphatidic Acid)

RN 565438-17-7 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-(diethoxyphosphinyl)-4-fluoro-2hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 7 
$$\underline{Z}$$
 (CH<sub>2</sub>) 7  $\underline{O}$  S  $\underbrace{CH_2}$  O  $\underbrace$ 

RN 565438-21-3 CAPLUS

Hexadecanoic acid, (2S)-4-(diethoxyphosphinyl)-4-fluoro-2-hydroxybutyl CN ester (CA INDEX NAME)

Absolute stereochemistry.

RN 565453-74-9 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2R)-4-(diethoxyphosphinyl)-4-fluoro-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 7 
$$\underline{Z}$$
 (CH<sub>2</sub>) 7  $\underline{O}$   $R$   $P$   $O$  EtO

RN 565453-75-0 CAPLUS

CN Hexadecanoic acid, (2R)-4-(diethoxyphosphinyl)-4-fluoro-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry.

IT 565438-23-5P 565438-27-9P 565453-76-1P

565453-77-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis and platelet aggregation activation of monofluorinated and  $\alpha$ -fluoromethylene phosphonate analogs of lysophosphatidic Acid)

RN 565438-23-5 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 565438-27-9 CAPLUS

CN Hexadecanoic acid, (2S)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 565453-76-1 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2R)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 565453-77-2 CAPLUS

CN Hexadecanoic acid, (2R)-4-fluoro-2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 15 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2003:26755 CAPLUS <<LOGINID::20080519>>
- DN 138:354161
- TI A short synthesis of a novel nucleoside analog of Fosfomycin
- AU Hwang, Jae-Min; Jung, Kang-Yeoun
- CS Department of Environmental & Applied Chemistry, Kangnung National University, Kangwon-do, 210-702, S. Korea
- SO Bulletin of the Korean Chemical Society (2002), 23(12), 1848-1850 CODEN: BKCSDE; ISSN: 0253-2964
- PB Korean Chemical Society
- DT Journal

LA English

OS CASREACT 138:354161

AB A new nucleoside epoxyphosphonate has been prepared from cytidine as an analog of the antibiotic Fosfomycin in six steps in good yield. Its stereochem. has been confirmed by the crystal structure of the mandelate ester of the diol.

IT 310409-37-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure of; short synthesis of a novel nucleoside analog of Fosfomycin)

RN 310409-37-1 CAPLUS

CN Acetamide, N-[1-[(6S)-6-C-(diethoxyphosphinyl)-6-0-[(2R)-methoxyphenylacetyl]-2,3-0-(1-methylethylidene)- $\beta$ -D-allofuranosyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:810911 CAPLUS <<LOGINID::20080519>>

DN 138:39487

TI Synthesis of Chiral ( $\alpha,\alpha$ -Difluoroalkyl)phosphonate Analogs of (Lyso)phosphatidic Acid via Hydrolytic Kinetic Resolution

AU Xu, Yong; Prestwich, Glenn D.

CS Department of Medicinal Chemistry and Center for Cell Signaling, University of Utah, Salt Lake City, UT, 84108-1257, USA

SO Organic Letters (2002), 4(23), 4021-4024 CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREACT 138:39487

AB The hydrolytic kinetic resolution of 1,1-difluoro-3,4-epoxy-butylphosphonate using a chiral salen-Co complex was employed as a key step to obtain enantiomeric diols in 99% ee as key intermediates. The enantiomerically homogeneous ( $\alpha$ , $\alpha$ -difluoroalkyl)phosphonates were obtained after selective esterification and deprotection of the corresponding phosphonates. These compds. are novel phosphatase-resistant analogs of lysophosphatidic acid and phosphatidic acid.

IT 478529-57-6P 478798-18-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of chiral  $(\alpha, \alpha$ -Difluoroalkyl)phosphonate

(lyso)phosphatidic acid analogs via hydrolytic kinetic resolution as a key step)

RN 478529-57-6 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4-(diethoxyphosphinyl)-4,4-difluoro-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 478798-18-4 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2R)-4-(diethoxyphosphinyl)-4,4-difluoro-2-hydroxybutyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

Me (CH<sub>2</sub>) 7 
$$\underline{Z}$$
 (CH<sub>2</sub>) 7  $\underline{O}$   $R$   $P$   $O$  EtO

IT 478529-59-8P 478529-61-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of chiral  $(\alpha, \alpha$ -Difluoroalkyl)phosphonate

(lyso)phosphatidic acid analogs via hydrolytic kinetic resolution as a key step)

RN 478529-59-8 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2S)-4,4-difluoro-2-hydroxy-4-phosphonobutyl ester, disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

•2 Na

RN 478529-61-2 CAPLUS

CN 9-Octadecenoic acid (9Z)-, (2R)-4,4-difluoro-2-hydroxy-4-phosphonobutyl ester, disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

$$H_{2O3P}$$
  $F$   $O$   $O$   $(CH_2)_7$   $Z$   $(CH_2)_7$   $Me$ 

•2 Na

## RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 17 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:327914 CAPLUS <<LOGINID::20080519>>

DN 136:335270

 ${\tt TI}$  Lysophosphatidic acid analogs as agonists of the edg2 lysophosphatidic acid receptor

IN Erickson, James R.

PA Atairgin Technologies, Inc., USA

SO U.S., 15 pp. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡI	US 6380177	В1	20020430	US 2000-602235	20000623	
PRAI	US 1999-141078P	P	19990625			

OS MARPAT 136:335270

AB Applicant has probed the Edg2 lysophosphatidic acid (LPA) receptor with a series of LPA analogs to determine receptor activation. The present invention is drawn to a series of LPA analogs which function as Edg2 receptor agonists, and methods of using such compds. to activate the Edg2 receptor of the surface of a cell (yeast or mammalian). The compds. of the invention comprise a glycerol backbone with an Sn1 ester-linked saturated or unsatd. alkyl group, substitutions of the hydroxyl group (-OH) at carbon two of the glycerol backbone, and optional replacement of the phosphate di-anion with either a hydroxyl group or a dimethylated phosphate. These LPA analogs may find uses in cancer and neurol. disorders.

IT 418761-78-1 418761-79-2 418761-80-5 418761-81-6 418761-82-7 418761-83-8

418761-84-9 418761-85-0

RL: BSU (Biological study, unclassified); BIOL (Biological study) (lysophosphatidic acid analogs as agonists of edg2 lysophosphatidic acid receptor)

RN 418761-78-1 CAPLUS

CN Hexanoic acid, 2-hydroxy-3-phosphonopropyl ester (CA INDEX NAME)

RN 418761-79-2 CAPLUS

CN Decanoic acid, 2-hydroxy-3-phosphonopropyl ester (CA INDEX NAME)

RN 418761-80-5 CAPLUS

CN Tetradecanoic acid, 2-hydroxy-3-phosphonopropyl ester (CA INDEX NAME)

RN 418761-81-6 CAPLUS

CN Hexadecanoic acid, 2-hydroxy-3-phosphonopropyl ester (CA INDEX NAME)

RN 418761-82-7 CAPLUS

CN Octadecanoic acid, 2-hydroxy-3-phosphonopropyl ester (CA INDEX NAME)

RN 418761-83-8 CAPLUS

CN 9-Octadecenoic acid (9Z)-, 2-hydroxy-3-phosphonopropyl ester (CA INDEX NAME)

Double bond geometry as shown.

$$H_2O_3P$$
  $O$   $(CH_2)_7$   $Z$   $(CH_2)_7$   $Me$ 

RN 418761-84-9 CAPLUS

CN 9-Tetracosenoic acid, 2-hydroxy-3-phosphonopropyl ester, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 418761-85-0 CAPLUS

CN 9-Octadecenoic acid (9Z)-, 2-hydroxy-5-phosphonopentyl ester (CA INDEX NAME)

Double bond geometry as shown.

$$H_2O_3P$$
 (CH<sub>2</sub>)<sub>3</sub> OH (CH<sub>2</sub>)<sub>7</sub>  $Z$  (CH<sub>2</sub>)<sub>7</sub> Me

# RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 18 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2001:813776 CAPLUS <<LOGINID::20080519>>

Correction of: 1996:688985

DN 135:318650

Correction of: 126:60267

- TI Synthesis and enzymic evaluation of substrates and inhibitors of  $\beta\text{-glucuronidases}$
- AU Hoos, Roland; Jiang, Huixin; Vasella, Andrea; Weiss, Patrick
- CS Laboratorium Organische Chemie, ETH-Zurich, Zurich, CH-8092, Switz.
- SO Helvetica Chimica Acta (1996), 79(7), 1757-1784 CODEN: HCACAV; ISSN: 0018-019X
- PB Verlag Helvetica Chimica Acta
- DT Journal
- LA English

GΙ

AB The synthesis of the phosphonate and tetrazole analogs I [R = PO(ONa)2, CN4H; R1 = methylumbelliferyl, R2 = H] of 4-methylumbelliferyl glucuronide and their evaluation as substrates of several  $\beta$ -glucuronidases is reported. The syntheses of the L-ido-, D-gluco-, and D-galacto-configurated phosphonate analogs  $\alpha$ -II [R = PO(OMe)2, R1 = H; R = H, R1 = PO(OMe)2],  $\alpha/\beta$ -II [R = H, R1 = PO(OPh)2], and  $\alpha/\beta$ -III of protected glycuronates, the syntheses of phenylcarbamate I (R = CO2Na, R1R2 = NO2CNHPh) and its phosphono analog I (R = PO3Na2, R1R2 = NO2CNHPh), and their evaluation as inhibitors of the E. coli and bovine liver  $\beta$ -glucuronidases are also described.

IT 184874-59-7P 184874-60-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and enzymic evaluation of  $\beta\text{--glucuronidase}$  substrates and inhibitors)

RN 184874-59-7 CAPLUS

CN D-Xylose, 5-C-[bis(phenylmethoxy)phosphinyl]-, oxime, 2,3,4-triacetate, (1Z,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 184874-60-0 CAPLUS

CN D-Xylose, 5-C-[bis(phenylmethoxy)phosphinyl]-, oxime, 2,3,4-triacetate, (1E,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

- L7 ANSWER 19 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 2000:658697 CAPLUS <<LOGINID::20080519>>
- DN 134:17662
- TI Synthesis of phosphonate derivatives of uridine, cytidine, and cytosine arabinoside
- AU Jung, K.-Y.; Hohl, R. J.; Wiemer, A. J.; Wiemer, D. F.
- CS Department of Chemistry, University of Iowa, Iowa City, IA, 52242-1294, USA
- SO Bioorganic & Medicinal Chemistry (2000), 8(10), 2501-2509 CODEN: BMECEP; ISSN: 0968-0896
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- OS CASREACT 134:17662
- AB The vinyl phosphonate derivs. of uridine, cytidine, and cytosine arabinoside (ara-C) have been prepared through oxidation of appropriately protected nucleosides to the 5'-aldehydes and Wittig condensation with [(diethoxyphosphinyl)methylidine]triphenylphosphorane. Dihydroxylation of these vinyl phosphonates with an AD-mix reagent generated the new 5',6'-dihydroxy-6'-phosphonates. After hydrolysis of the phosphonate esters and the various protecting groups, the six phosphonic acids were tested for their ability to serve as substrates for the enzyme nucleotide monophosphate kinase and for their toxicity to K562 cells.
- IT 310409-33-7P 310409-37-1P
  - RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of phosphonate derivs. of uridine cytidine and cytosine arabinoside as substrate for nucleotide monophosphate kinase)
- RN 310409-33-7 CAPLUS
- CN Acetamide, N-[1-[(6S)-6-C-(diethoxyphosphinyl)-6-0-[(2S)-methoxyphenylacetyl]-2,3-0-(1-methylethylidene)- $\beta$ -D-allofuranosyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 310409-37-1 CAPLUS

CN Acetamide, N-[1-[(6S)-6-C-(diethoxyphosphinyl)-6-0-[(2R)-methoxyphenylacetyl]-2,3-0-(1-methylethylidene)- $\beta$ -D-allofuranosyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 20 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2000:153665 CAPLUS <<LOGINID::20080519>>

DN 132:322039

TI Synthesis of Glycophostones: Cyclic Phosphonate Analogues of Biologically Relevant Sugars

AU Hanessian, Stephen; Rogel, Olivier

CS Department of Chemistry, Universite de Montreal, Montreal, QC, H3C 3J7,

SO Journal of Organic Chemistry (2000), 65(9), 2667-2674 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

AB Analogs of L-fucose, N-acetyl-D-glucosamine, N-acetyl-D-mannosamine, and N-acetyl neuraminic acid in which the anomeric carbon atom was replaced by a phosphonyl group (phostones or cyclic phosphonates) were synthesized by stereocontrolled methods relying on the Abramov reaction.

IT 266677-44-5P 266677-45-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of glycophostones: cyclic phosphonate analogs of biol. relevant sugars)

RN 266677-44-5 CAPLUS

CN D-glycero-D-gluco-Heptitol, 3-(acetylamino)-3-deoxy-1-C- (dimethoxyphosphinyl)-2,5,6,7-tetrakis-O-(phenylmethyl)-, 4-(methyl ethanedioate), (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 266677-45-6 CAPLUS

CN D-glycero-D-gluco-Heptitol, 3-(acetylamino)-3-deoxy-1-C- (dimethoxyphosphinyl)-2,5,6,7-tetrakis-O-(phenylmethyl)-, 4-(methyl ethanedioate), (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

## RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 21 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
- AN 1999:571300 CAPLUS <<LOGINID::20080519>>
- DN 131:310828
- TI Synthesis of a phostone glycomimetic of the endothelin converting enzyme inhibitor phosphoramidon
- AU Hanessian, Stephen; Rogel, Olivier
- CS Department of Chemistry, Universite de Montreal, Montreal, QC, H3C 3J7, Can.
- SO Bioorganic & Medicinal Chemistry Letters (1999), 9(16), 2441-2446 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- AB The phostone analog of phosphoramidon, an inhibitor of endothelin converting enzyme, was synthesized from L-rhamnose. Coupling of the cyclic phosphonic acid with the dipeptide H-Leu-Trp-OMe gave, after deprotection and purification by reverse-phase HPLC, the desired phostone which exhibited an IC50 of 5.05  $\pm$  2.7  $\mu M$ .
- IT 247579-99-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of in the synthesis of a phostone glycomimetic of the endothelin converting enzyme inhibitor phosphoramidon)

RN 247579-99-3 CAPLUS

CN L-Arabinitol, 5-deoxy-1-C-(dimethoxyphosphinyl)-, 2,3-diacetate 4-formate (CA INDEX NAME)

Absolute stereochemistry.

#### RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 22 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1998:269301 CAPLUS <<LOGINID::20080519>>

DN 128:257012

TI Rh-DuPHOS-Catalyzed Enantioselective Hydrogenation of Enol Esters. Application to the Synthesis of Highly Enantioenriched  $\alpha$ -Hydroxy Esters and 1,2-Diols

AU Burk, Mark J.; Kalberg, Christopher S.; Pizzano, Antonio

CS P. M. Gross Chemical Laboratory Department of Chemistry, Duke University, Durham, NC, 27706, USA

SO Journal of the American Chemical Society (1998), 120(18), 4345-4353 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 128:257012

The asym. hydrogenation of  $\alpha$ -(acetyloxy)- and  $\alpha$ -(benzoyloxy)acrylates, catalyzed by cationic rhodium-DuPHOS complexes, has been examined A wide range of substrates were prepared via a convenient Horner-Emmons condensation protocol and subsequently hydrogenated under mild conditions (60 psi of H2) at substrate-to-catalyst ratios of 500. Overall, enol ester substrates were reduced by the cationic Et-DuPHOS-Rh catalysts with very high levels of enantioselectivity (93-99% ee). Importantly, substrates bearing  $\beta$ -substituents could be employed as E/Z isomeric mixts. with no detrimental effect on the selectivity. Labeling studies indicated that no significant E/Z isomerization of the substrates occurs during the course of these reactions. Details concerning optimization of the reaction, interesting solvent effects, and deprotection procedures for the synthesis of highly enantioenriched  $\alpha$ -hydroxy esters and 1,2-diols also are provided.

IT 205264-44-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(rhodium-DuPHOS-catalyzed asym. hydrogenation of enol esters)

RN 205264-44-4 CAPLUS

CN Acetic acid, (acetyloxy)(diethoxyphosphinyl)- (9CI) (CA INDEX NAME)

#### RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 23 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1998:56603 CAPLUS <<LOGINID::20080519>>

DN 128:140772

TI Asymmetric dihydroxylation of 1-acyloxy-2(E)-alkenylphosphonates with AD-mix reagents. Effects of 1-acyloxy functional groups on the asymmetric dihydroxylation

AU Yokomatsu, Tsutomu; Yamagishi, Takehiro; Sada, Tomoyuki; Suemune, Kenji; Shibuya, Shiroshi

CS Sch. Pharm., Tokyo Univ. Pharmacy Life Sci., Hachioji, 192-03, Japan

SO Tetrahedron (1998), 54(5/6), 781-790 CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 128:140772

AB Asym. dihydroxylation (AD) of a racemic mixture of 1-acyloxy-2(E)-alkenylphosphonates with AD-mix- $\alpha$  or - $\beta$  reagents (K3Fe(CN)6/K2OsO4/MeSO2NH2/K2CO3/quinuclidine) was examined. The kinetic rate of dihydroxylation was highly dependent upon the configuration of the 1-acyloxy functional group as well as the nature of substituents at the 3-position. The reaction of a racemic mixture of di-Et (E)-3-phenyl-1-acetyloxy-2-propenylphosphonate with an AD-mix- $\beta$  reagent preferentially dihydroxylated the R-enantiomer to leave an unreacted S-enantiomer of high enantiomeric purity. Double diastereoselection of the resolved di-Et 3-phenyl-1-acetyloxy-2(E)-propenylphosphonate in dihydroxylation was also examined

IT 202004-61-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with dimethoxypropane to give acetonide derivative)

RN 202004-61-3 CAPLUS

CN Phosphonic acid, [1-(acetyloxy)-2,3-dihydroxy-3-phenylpropyl]-, diethyl ester,  $[1R-(1R^*,2S^*,3R^*)]-$  (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 202004-63-5P

RN 202004-63-5 CAPLUS

CN Phosphonic acid, [1-(acetyloxy)-2,3-dihydroxy-3-phenylpropyl]-, diethyl ester,  $[1R-(1R^*,2R^*,3S^*)]-$  (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 24 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1996:688985 CAPLUS <<LOGINID::20080519>>

DN 126:60267

TI Synthesis and enzymic evaluation of substrates and inhibitors of  $\beta\text{-glucuronidases}$ 

AU Hoos, Roland; Huixin, Jiang; Vasella, Andrea; Weiss, Patrick

CS Laboratorium Organische Chemie, ETH-Zurich, Zurich, CH-8092, Switz.

SO Helvetica Chimica Acta (1996), 79(7), 1757-1784 CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB The synthesis of the phosphonate and tetrazole analogs I [R = PO(ONa)2, CN4H; R1 = methylumbelliferyl, R2 = H] of 4-methylumbelliferyl glucuronide and their evaluation as substrates of several  $\beta$ -glucuronidases is reported. The syntheses of the L-ido-, D-gluco-, and D-galacto-configurated phosphonate analogs  $\alpha$ -II [R = PO(OMe)2, R1 = H; R = H, R1 = PO(OMe)2],  $\alpha/\beta$ -II [R = H, R1 = PO(OPh)2], and  $\alpha/\beta$ -III of protected glycuronates, the syntheses of phenylcarbamate I (R = CO2Na, R1R2 = NO2CNHPh) and its phosphono analog I (R = PO3Na2, R1R2 = NO2CNHPh), and their evaluation as inhibitors of the E. coli and bovine liver  $\beta$ -glucuronidases are also described.

IT 184874-59-7P 184874-60-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and enzymic evaluation of  $\beta\text{--glucuronidase}$  substrates and inhibitors)

RN 184874-59-7 CAPLUS

CN D-Xylose, 5-C-[bis(phenylmethoxy)phosphinyl]-, oxime, 2,3,4-triacetate, (1Z,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 184874-60-0 CAPLUS

CN D-Xylose, 5-C-[bis(phenylmethoxy)phosphinyl]-, oxime, 2,3,4-triacetate, (1E,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L7 ANSWER 25 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1996:672866 CAPLUS <<LOGINID::20080519>>

DN 125:339157

TI Preparation of lysophosphatidic acids for treating hyperproliferative conditions

IN Piazza, Gary A.; Mazur, Adam W.

PA The Procter & Gamble Company, USA

SO U.S., US14 pp., Cont. of U. S. Ser. No. 980,814, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	US 5565439	A	19961015	US 1994-334888	19941104		
PRAI	US 1992-980814	В1	19921124				

OS MARPAT 125:339157

AB The invention involves a method for treating hyperproliferative conditions (no data ) in mammalian epithelial cells, comprising administering a lysophosphatidic acid derivative (preparation given) RC(:X)XCH2CHZCH2YPO3H2 or its

cyclic derivative [Y = 0 or CH2; Z = H, XH or halo; X = 0 or S; R = (un) substituted (un) saturated, straight or branched C11-23 alkyl]. 1-Oleoylglycerol-3-phosphate is an example. The compns. are usable for the treatment of skin cancer, psoriasis, dandruff, etc.

IT 146491-10-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate in preparation of lysophosphatidic acid derivative for treating

skin hyperproliferative conditions)

RN 146491-10-3 CAPLUS

CN Tetradecanoic acid, 4-[bis(1-methylethoxy)phosphinyl]-2-hydroxybutyl ester (CA INDEX NAME)

IT 146491-11-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation as agent for treating skin hyperproliferative conditions)

RN 146491-11-4 CAPLUS

CN Tetradecanoic acid, 2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

L7 ANSWER 26 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1996:604558 CAPLUS <<LOGINID::20080519>>

DN 125:329253

TI Synthesis and antiviral activity of new phosphonobutoxypurines

Ι

ΙI

AU Harnden, Michael R.; Serafinowska, Halina T.

CS SmithKline Beecham Pharmaceuticals, Epsom, KT18 5XQ, UK

SO Bioorganic & Medicinal Chemistry Letters (1996), 6(18), 2215-2218 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier

DT Journal

LA English

GΙ

AB The 9-(4-phosphonobutoxy) guanines I (R2 = H, CH2OH) and the the 9-(4-phosphonobutoxy) purinamines II (Y = NH2, H; R2 = H, CH2OH) were prepared and evaluated as antiviral agents. 9-(4-Phosphonobutoxy) guanine

displayed potent and selective activity against  ${\tt HIV-1}$  in peripheral blood  ${\tt lymphocytes.}$ 

IT 133866-78-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (phosphonobutoxy) purines and (phosphonobutoxy) guanines as virucides)

RN 133866-78-1 CAPLUS

CN Phosphonic acid, [4-(acetyloxy)-3-(hydroxymethyl)butyl]-, diethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{OH} & \text{O} \\ | & || \\ \text{AcO-CH}_2-\text{CH-CH}_2-\text{CH}_2-\text{P-OEt} \\ | & | \\ \text{OEt} \end{array}$$

L7 ANSWER 27 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1996:589339 CAPLUS <<LOGINID::20080519>>

DN 125:301519

TI Lipase-catalyzed enantioselective acylation of prochiral 2-( $\omega$ -phosphono)alkyl-1,3-propanediols: application to the enantioselective synthesis of  $\omega$ -phosphono- $\alpha$ -amino acids

AU Yokomatsu, Tsutomu; Sato, Mutsumi; Shibuya, Shiroshi

CS School Pharmacy, Tokyo University Pharmacy Life Science, Tokyo, 192-03, Japan

SO Tetrahedron: Asymmetry (1996), 7(9), 2743-2754 CODEN: TASYE3; ISSN: 0957-4166

PB Elsevier

DT Journal

LA English

OS CASREACT 125:301519

GΙ

HO 
$$Z-PO3Et_2$$
 I  $HO_2C$   $(CH_2)_nPO3Et_2$  II

AB Lipase PS catalyzed acetylation of prochiral 2-( $\omega$ -phosphono)alkyl-1,3-propanediols (HOCH2)2CH-Z-PO3Et2 (Z = CH2, CH2CH2, CH2CF2) was found to proceed with high enantioselectivity. The applications of phosphonic chirons I thus obtained were illustrated by the stereocontrolled synthesis of  $\omega$ -phosphono- $\alpha$ -amino acids such as II (n = 1, 2) and III.

IT 182691-03-8P 182691-04-9P 182691-05-0P RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological

Absolute stereochemistry. Rotation (+).

RN 182691-04-9 CAPLUS

CN Phosphonic acid, [4-(acetyloxy)-3-(hydroxymethyl)butyl]-, diethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 182691-05-0 CAPLUS

CN Phosphonic acid, [(3R)-4-(acetyloxy)-1,1-difluoro-3-(hydroxymethyl)butyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 182691-06-1P 182691-08-3P 182691-09-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(lipase-catalyzed stereoselective acylation of prochiral

(phosphonoalkyl)propanediols in preparation of phosphono amino acids)

RN 182691-06-1 CAPLUS

CN Propanoic acid, 3-(acetyloxy)-2-[(diethoxyphosphinyl)methyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 182691-08-3 CAPLUS

CN Butanoic acid, 2-[(acetyloxy)methyl]-4-(diethoxyphosphinyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 182691-09-4 CAPLUS

CN Butanoic acid, 2-[(acetyloxy)methyl]-4-(diethoxyphosphinyl)-4,4-difluoro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L7 ANSWER 28 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1995:537220 CAPLUS <<LOGINID::20080519>>

DN 123:6237

OREF 123:1302h,1303a

TI Lysophosphatidic acid-induced Ca2+ mobilization in human A431 cells: structure-activity analysis

AU Jalink, Kees; Hengeveld, Trudi; Mulder, Sipko; Postma, Friso R.; Simon, Marie Francoise; Chap, Hugues; van der Marel, Gijs A.; van Boom, Jacques H.; van Blitterswijk, Wim J.; Moolenaar, Wouter H.

CS Div. Cellular Biochemistry, Netherlands Cancer Inst., Amsterdam, 1066 CX, Neth.

SO Biochemical Journal (1995), 307(2), 609-16 CODEN: BIJOAK; ISSN: 0264-6021

PB Portland Press

DT Journal

LA English

AB Lysophosphatidic acid (LPA; 1-acyl-sn-glycero-3-phosphate) is a platelet-derived lipid mediator that activates its own G-protein-coupled receptor to trigger phospholipase C-mediated Ca2+ mobilization and other effector pathways in numerous cell types. In this study the authors have examined the structural features of LPA that are important for activation of the Ca2+-mobilizing receptor in human A431 carcinoma cells, which show an EC50 for oleoyl-LPA as low as 0.2 nM. When the acyl chain at the sn-1

position is altered, the rank order of potency is oleoyl-LPA > arachidonoyl-LPA > linolenoyl-LPA > linoleoyl-LPA > stearoyl-LPA = palmitoyl-LPA > myristoyl-LPA. The shorter-chain species, lauroyl- and decanoyl-LPA, show little or no activity. Ether-linked LPA (1-O-hexadecyl-sn-glycero-3-phosphate) is somewhat less potent than the corresponding ester-linked LPA; its stereoisomer is about equally active. Deletion of the glycerol backbone causes a 1000-fold decrease in potency. Replacement of the phosphate group in palmitoyl-LPA by a hydrogen- or methyl-phosphonate moiety results in complete loss of activity. A phosphonate analog with a methylene group replacing the oxygen at sn-3 has strongly decreased activity. All three phosphonate analogs induce cell lysis at doses  $>15~\mu\mathrm{M}$ . Similarly, the Me and Et esters of palmitoyl-LPA are virtually inactive and become cytotoxic at micromolar doses. None of the LPA analogs tested has antagonist activity. Sphingosine 1-phosphate, a putative messenger with some structural similarities to LPA, elicits a transient rise in intracellular [Ca2+] only at micromolar doses; however, cross-desensitization expts. indicate that sphingosine 1-phosphate does not act through the LPA receptor. The results indicate that, although many features of the LPA structure are important for optimal activity, the phosphate group is most critical, suggesting that this moiety is directly involved in receptor activation.

IT 163595-65-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(lysophosphatidate induction of calcium mobilization in human A431 cells in relation to structure)

RN 163595-65-1 CAPLUS

CN Hexadecanoic acid, 2-hydroxy-4-phosphonobutyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 29 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1994:185889 CAPLUS <<LOGINID::20080519>>

DN 120:185889

OREF 120:32701a,32704a

TI Studies on the active site of dihydroxy-acid dehydratase

AU Flint, Dennis H.; Nudelman, Abraham

CS Exp. Stn., E. I. du Pont de Nemours & Co., Wilmington, DE, 19880-0328, USA

SO Bioorganic Chemistry (1993), 21(4), 367-85 CODEN: BOCMBM; ISSN: 0045-2068

DT Journal

LA English

AB Several classes of substrate analogs of dihydroxy-acid dehydratase have been tested as inhibitors of this enzyme in an attempt to characterize its binding site and find what modifications in substrate structure lead to an affinity higher than that of the natural substrates. The substrate analogs were tested on dihydroxy-acid dehydratase from both spinach and Escherichia coli. One modification of the substrate that led to as much as a 1000-fold increase in binding affinity was replacement of the 3-hydroxyl group with a thiol. It has been shown previously that the

3-hydroxyl group of the substrate becomes a ligand for one Fe of the Fe-S clusters of these enzymes on binding to their active sites. It seems likely then that the tighter binding of the thiol containing analogs is due to the thiol group becoming a ligand to an iron of the Fe-S clusters of these enzymes. A second modification in substrate that led to as much as 1000-fold increase in binding affinity was the addition of a large lipophilic group. This suggests there is a large hydrophobic pocket or hydrophobic surface near the active site of dihydroxy-acid dehydratase. A modification in substrate that led to as much as a 50-fold increase in binding was the replacement of the carboxyl group of the substrate with phosphonate; however, this increase was limited to substrate analogs without a polar functionality on the carbon  $\beta$  to the phosphonate group. Bromopyruvate was found to irreversibly inactivate dihydroxy-acid dehydratase. Each good inhibitor the authors found was active on spinach dihydroxy-acid dehydratase and E. coli dihydroxy-acid dehydratase to a similar extent suggesting the active sites of the enzymes from these two organisms are similar. Some of the better inhibitors described in this report have mild herbicidal activity.

ΙT 153733-58-5

RL: BIOL (Biological study)

(reflux of)

RN 153733-58-5 CAPLUS

Phosphonic acid, [2-(acetyloxy)-1-hydroxy-2-methylpropyl]- (9CI) (CA CN INDEX NAME)

L7 ANSWER 30 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

ΑN 

DN 118:213409

OREF 118:36807a,36810a

Phosphonolipids. Synthesis of 1-hydroxy-3-acyloxypropylphosphonic acids and their derivatives

ΑU Alekseichuk, I. A.; Ofitserov, E. N.; Konovalova, I. V.

Kazan. Gos. Univ., Kazan, Russia CS

SO Zhurnal Obshchei Khimii (1992), 62(4), 786-96 CODEN: ZOKHA4; ISSN: 0044-460X

DТ Journal

LA Russian

CASREACT 118:213409 OS

GΙ

AB Addition of (EtO)2P(O)H to MeCOCH2CH2OR (R = Ac) gave (EtO)2P(O)C(OH)MeCH2CH2OAc and the cyclic phospholane I via an Abramov reaction. Similarly, MeCOCH2CH2OR (R = Ac, C11H23CO) and (EtO)2POSiMe3 gave (EtO)2P(O)C(OSiMe3)MeCH2CH2OR which underwent hydrolysis to give (EtO)2P(O)C(OH)MeCH2CH2OR. Treating MeCOCH2CH2OR (R = Ac, C11H23CO) with P(OSiMe3)3 gave (Me3SiO)2P(O)C(OSiMe3)MeCH2CH2OR which were treated with aqueous bases B (B = LiOH, morpholine, Et3N, heptylamine, diethanolamine, and Me3CNH2) to give 88-96% RCO2CH2CH2C(OH)MeP(O)O22-(BH)22+ salts some of which have a liquid crystalline phase.

IT 146828-84-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and rearrangement of)

RN 146828-84-4 CAPLUS

CN Phosphonic acid, [3-(acetyloxy)-1-hydroxy-1-methylpropyl]-, bis(2,2,3,3-tetrafluoropropyl) ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \mathsf{F}_2\mathsf{CH}-\mathsf{CF}_2-\mathsf{CH}_2-\mathsf{O}-\mathsf{P}-\mathsf{O}-\mathsf{CH}_2-\mathsf{CF}_2-\mathsf{CHF}_2 \\ | \\ \mathsf{Me}-\mathsf{C}-\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{OAc} \\ | \\ \mathsf{OH} \end{array}$$

•2 Li

RN 146813-06-1 CAPLUS

CN Dodecanoic acid, 3-hydroxy-3-phosphonobutyl ester, dilithium salt (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{O} \\ | & | \\ \text{Me-C-CH}_2\text{--CH}_2\text{---C-(CH}_2)_{10}\text{---Me} \\ | & \\ \text{PO}_3\text{H}_2 \end{array}$$

●2 Li

RN 146813-07-2 CAPLUS

CN Dodecanoic acid, 3-hydroxy-3-phosphonobutyl ester, dipotassium salt (9CI) (CA INDEX NAME)

●2 K

RN 146828-75-3 CAPLUS

RN 146828-82-2 CAPLUS

CN Dodecanoic acid, 3-(dimethoxyphosphinyl)-3-hydroxybutyl ester (CA INDEX NAME)

RN 147217-28-5 CAPLUS

CN Phosphonic acid, [3-(acetyloxy)-1-hydroxy-1-methylpropyl]-, compd. with

morpholine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147217-27-4 CMF C6 H13 O6 P

CM 2

CRN 110-91-8 CMF C4 H9 N O

RN 147217-29-6 CAPLUS

CN Phosphonic acid, [3-(acetyloxy)-1-hydroxy-1-methylpropyl]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147217-27-4 CMF C6 H13 O6 P

CM 2

CRN 121-44-8 CMF C6 H15 N

RN 147217-30-9 CAPLUS

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Phosphonic acid, [3-(acetyloxy)-1-hydroxy-1-methylpropyl]-, compd. with
CN
     1-heptanamine (1:1) (9CI) (CA INDEX NAME)
     CM
           1
     CRN 147217-27-4
     CMF C6 H13 O6 P
    ОН
Me-C-CH_2-CH_2-OAc
    PO3H2
     CM
           2
     CRN 111-68-2
     CMF C7 H17 N
Me^- (CH<sub>2</sub>)<sub>6</sub>-NH<sub>2</sub>
     147217-31-0 CAPLUS
RN
     Phosphonic acid, [3-(acetyloxy)-1-hydroxy-1-methylpropyl]-, compd. with
CN
     2,2'-iminobis[ethanol] (1:1) (9CI) (CA INDEX NAME)
     CM
           1
     CRN 147217-27-4
     CMF C6 H13 O6 P
    ОН
\text{Me-C-CH}_2\text{--CH}_2\text{--}\text{OAc}
    PO3H2
     СМ
           2
     CRN 111-42-2
     CMF C4 H11 N O2
{\tt HO-CH_2-CH_2-NH-CH_2-CH_2-OH}
RN
     147217-32-1 CAPLUS
     Phosphonic acid, [3-(acetyloxy)-1-hydroxy-1-methylpropyl]-, compd. with
     2-(methylamino)ethanol (1:1) (9CI) (CA INDEX NAME)
```

CM 1

CRN 147217-27-4 CMF C6 H13 O6 P

$$\begin{array}{c} & \text{OH} \\ | \\ \text{Me-C-CH}_2\text{-CH}_2\text{-OAc} \\ | \\ \text{PO}_3\text{H}_2 \end{array}$$

CM 2

CRN 109-83-1 CMF C3 H9 N O

HO-CH2-CH2-NH-CH3

RN 147217-34-3 CAPLUS

CN Dodecanoic acid, 3-hydroxy-3-phosphonobutyl ester, compd. with morpholine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147217-33-2 CMF C16 H33 O6 P

CM 2

CRN 110-91-8 CMF C4 H9 N O

RN 147217-35-4 CAPLUS

CN Dodecanoic acid, 3-hydroxy-3-phosphonobutyl ester, compd. with 1-heptanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147217-33-2 CMF C16 H33 O6 P

CM 2

CRN 111-68-2 CMF C7 H17 N

 $Me^{-(CH_2)}6^{-NH_2}$ 

RN 147217-36-5 CAPLUS

CN Dodecanoic acid, 3-hydroxy-3-phosphonobutyl ester, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147217-33-2 CMF C16 H33 O6 P

CM 2

CRN 75-64-9 CMF C4 H11 N

RN 147217-37-6 CAPLUS

CN Dodecanoic acid, 3-hydroxy-3-phosphonobutyl ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147217-33-2

CMF C16 H33 O6 P

CM 2

CRN 121-44-8 CMF C6 H15 N

RN 147217-38-7 CAPLUS

CN Dodecanoic acid, 3-hydroxy-3-phosphonobutyl ester, compd. with 2-(methylamino)ethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 147217-33-2 CMF C16 H33 O6 P

CM 2

CRN 109-83-1 CMF C3 H9 N O

$${\tt HO-CH_2-CH_2-NH-CH_3}$$

RN 148595-50-0 CAPLUS

CN Dodecanoic acid, 3-(diethoxyphosphinyl)-3-hydroxybutyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ || \\ \text{EtO-P-OEt} \\ | \\ \text{Me-C-CH}_2\text{-CH}_2\text{-O-C-(CH}_2)_{10}\text{-Me} \\ || \\ \text{OH} \end{array}$$

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L7 ANSWER 31 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
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AN 1993:175516 CAPLUS <<LOGINID::20080519>>

DN 118:175516

OREF 118:29963a,29966a

 ${\tt TI}$  Use of lysophosphatidic acids in cosmetics for the treatment of skin wrinkles

IN Piazza, Gary Anthony; Mazur, Adam Wieslaw

PA Procter and Gamble Co., USA

SO PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.					KIND DATE			APPLICATION NO.							DATE		
ΡI	WO 9221323			A1 19921210			WO 1992-US4415						19920518					
		W:	ΑU,	BB,	BG,	BR,	CA,	CS,	FΙ,	HU,	JΡ,	KP,	KR,	LK,	MG,	MN,	MW,	NO,
			PL,	RO,	RU,	SD												
		RW:	AT,	BE,	BF,	ВJ,	CF,	CG,	CH,	CI,	CM,	DE,	DK,	ES,	FR,	GΑ,	GB,	GN,
			GR,	ΙΤ,	LU,	MC,	ML,	MR,	NL,	SE,	SN,	TD,	TG					
	US 5238965			А		19930824 US 1991-708270					19910531							
	AU	9221	590			Α		19930108 AU 1992-21590					19920518					
	CN 1068034			A	19930120			CN 1992-105123						19920530				
	US	5521	223			A		1996	0528	,	US 1	993-	6166	0		1	9930	513
PRAI	US	1991	-708	270		A		1991	0531									
	WO	1992	-US4	415		Α		1992	0518									
OS GI	MAI	RPAT	118:	1755	16													

AB Cosmetics containing lysophosphatidic acid RC(:X)XCH2CH(XH)CH2YPO3H2 or cyclic derivs. thereof (I) (R = C12-23 alkyl; X = O, S; Y = O, CH2) are used for the treatment of skin wrinkles. Thus, 1-hexadecanoyl-sn-glycerol was reacted with phosphorous oxychloride to obtain 1-O-hexadecanoyl-1,2-cyclic sn-glycerolphosphate. A topical solution contained EtOH 99.87, and oleyl phosphatidic acid 0.13%.

IT 146491-10-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of)

RN 146491-10-3 CAPLUS

CN Tetradecanoic acid, 4-[bis(1-methylethoxy)phosphinyl]-2-hydroxybutyl ester (CA INDEX NAME)

IT 146491-11-4P

RL: PREP (Preparation)

(preparation of, antiwrinkle cosmetics containing)

RN 146491-11-4 CAPLUS

CN Tetradecanoic acid, 2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

L7 ANSWER 32 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1992:255351 CAPLUS <<LOGINID::20080519>>

DN 116:255351

OREF 116:43283a,43286a

TI Regio- and stereoselective enzymic esterification of glycerol and its derivatives

AU Mazur, Adam W.; Hiler, George D., II; Lee, Susannie S. C.; Armstrong, Molly P.; Wendel, Jack D.

CS Miami Valley Lab., Procter and Gamble Co., Cincinnati, OH, 45239-8707, USA

SO Chemistry and Physics of Lipids (1991), 60(2), 189-99 CODEN: CPLIA4; ISSN: 0009-3084

DT Journal

LA English

AB A methodol. for regio- and stereoselective preparation of acyl glycerol derivs. is presented. It offers easy access to specific 1,2-, 1,3-diglycerides and triglycerides as well as alkyl glycerol esters, phospholipids, and glycolipids. These compds. are prepared by esterification of the corresponding glycerol derivs. such as 2-monoglycerides, alkyl glycerols, glyceryl glycosides, glyceryl phosphate esters, or unsubstituted glycerol. The regio- and stereoselectivity in the esterification is achieved by using fatty acid anhydrides and an enzymic catalyst, 1,3-specific lipase. NMR methods for determining the regio- and stereoselectivity of esterification are discussed.

IT 141590-47-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 141590-47-8 CAPLUS

CN Tetradecanoic acid, 3-[bis(1-methylethoxy)phosphinyl]-2-hydroxypropyl
 ester (CA INDEX NAME)

L7 ANSWER 33 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1991:511428 CAPLUS <<LOGINID::20080519>>

DN 115:111428

OREF 115:19041a,19044a

TI Potent Gi-mediated inhibition of adenylyl cyclase by a phosphonate analog of monooleylphosphatidate

AU Proll, Melissa A.; Clark, Richard B.

CS Health Sci. Cent., Univ. Texas, Houston, TX, 77225, USA

SO Molecular Pharmacology (1991), 39(6), 740-4 CODEN: MOPMA3; ISSN: 0026-895X

DT Journal

LA English

AB It was previously demonstrated that monooleylphosphatidate (MOPA) and phosphatidate inhibit adenylyl cyclase in cultured fibroblasts. In this study, the specificity of the phospholipid effect was probed by anal. of the effect of phosphonate analogs of these phospholipids on adenylyl cyclase in C6 glioma cells. The MOPA phosphonate analog inhibited adenylyl cyclase, but the comparable phosphonate analog of phosphatidate was ineffective. The IC50 for inhibition of adenylyl cyclase by the MOPA phosphonate analog was similar to that of MOPA, the maximal inhibitions were comparable (approx. 45% inhibition of hormone-stimulated adenylyl cyclase), and the effects of both appeared to be mediated by Gi, because treatment with islet-activating protein reduced the inhibition to 5-10%.

IT 64032-88-8

RL: BIOL (Biological study)

(adenylyl cyclase inhibition by)

RN 64032-88-8 CAPLUS

CN Hexadecanoic acid, 2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

L7 ANSWER 34 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1991:429829 CAPLUS <<LOGINID::20080519>>

DN 115:29829

OREF 115:5261a,5264a

TI Preparation of sugar phosphonates as antidiabetics

PA American Cyanamid Co., USA

SO Jpn. Kokai Tokkyo Koho, 37 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.					KIN	D	DATE			APE	PLICA	DATE				
						_											
PΙ	JP	0211	1783			А		1990	0424		JP	1989-	-2095	16		19890	811
	US	4945	158			Α		1990	0731		US	1988-	-2323	33		19880	812
	EP 372157				A1		1990	19900613		EP 1989-11		-1118	.1838		19890	629	
		R:	ΑT,	BE,	CH,	DE,	ES	, FR,	GB,	GR,	I]	C, LI	, NL,	SE			

PRAI US 1988-232333 A 19880812

OS MARPAT 115:29829

GI

AB The title compds. [I; A, B = C1-4 alkylene, C2-4 hydroxyalkylene; R = H, OH, C1-4 (hydroxy)alkyl, C2-4 dihydroxyalkyl, etc.; R1-R4 = H, C1-13 alkyl C3-6 cycloalkyl, (substituted) Ph, isoalkyl, etc.] are prepared Reduction of ester II (Bzl = PhCH2, R5 = CO2Et) (preparation given) with LiAlH4 in Et20 under Ar gave a mixture of D-gluco- and D-manno-heptitol II (R5 = CH2OH), which was oxidized with Cr2O3 in CH2Cl2-pyridine under Ar to give a mixture of D-gluco- and D-manno-heptose II (R5 = CHO) (III). Wittig reaction of III with Ph3P:CHP(O)(OPh)2 in MePh gave a mixture of D-gluco- and D-manno-octenitol II [R5 = CH:CHP(0)(OPh)2], which (1.27 g) was hydrogenated over 10% Pd-C to give, after separation by flash chromatog., 270 mg D-gluco-octitol II [R5 = CH2CH2P(O)(OPh)2] (IV) and 240 mg D-manno isomer. IV (215 mg) was phosphorylated with ClP(O)(OPh)2 in pyridine to give 232 mg D-gluco-I [A = CH2, B = (CH2)3 , R = H, R1-R4 = Ph]. Also prepared were 50 addnl. I and intermediates. I showed ED50 of 4-27  $\mu M$  in stimulation of 1-phosphofructokinase and IC50 of 58-602  $\mu \text{M}$  in inhibition of fructose 1,6-diphosphatase.

IT 130372-53-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of antidiabetics)

RN 130372-53-1 CAPLUS

CN D-Fructose, 1-deoxy-1-(diethoxyphosphinyl)-3,4-bis-0-(phenylmethyl)-, 6-acetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 35 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1991:229308 CAPLUS <<LOGINID::20080519>>

DN 114:229308

OREF 114:38701a,38704a

TI Preparation of 9-(phosphonoalkoxy)purines as virucides

IN Harnden, Michael R.; Duckworth, David M.; Serafinowska, Halina T.

PA Beecham Group PLC, UK

SO Eur. Pat. Appl., 36 pp. CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1												
Ε	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE							
-												
PI E	EP 404296	A1	19901227	EP 1990-303178	19900326							
	R: CH, DE, FR,	GB, IT	, LI, NL									
J	US 5166198	A	19921124	US 1990-500718	19900328							
	JP 02286682	A	19901126	JP 1990-81482	19900330							
PRAI (	GB 1989-7173	A	19890330									
OS N	MARPAT 114:229308											
GI												

- The title compds. [I; R1 = OH, amino; R2 = H, amino; R3 = H, CH2OH, acyloxymethyl; R4 = H; when R3 = H and Z = bond, CH2, then R4 = OH, acyloxy, CH2OH, acyloxymethyl; R6, R7 = H, alkyl, (substituted) Ph; Z = bond, CHR8; R8 = H; when R3 = R4 = H, then R8 = OH, acyloxy, CH2OH, acyloxymethyl], were prepared Thus, 6-chloro-9-[4- (diethoxyphosphoryl)butoxy]-2-formamidopurine [preparation from 4,6-dichloro-2,5-diformamidopyrimidine and di-Et 4- (aminooxy)butylphosphonate given] was stirred 5 h in 80% HCO2H at 80° to give 76% 9-[4-(diethoxyphosphoryl)butoxy]guanine. The latter in DMF was treated with Me3SiBr to give 64% title compound which had an IC50 of 62  $\mu \rm g/mL$  against Herpes simplex HFEM in Vero cells.
- CN Phosphonic acid, [4-(acetyloxy)-3-(hydroxymethyl)butyl]-, diethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 36 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1990:531820 CAPLUS <<LOGINID::20080519>>

DN 113:131820

OREF 113:22383a,22386a

TI The total synthesis of oleandomycin

AU Tatsuta, Kuniaki; Ishiyama, Takashi; Tajima, Shuichi; Koguchi, Yoshihito; Gunji, Hiroki

CS Dep. Appl. Chem., Keio Univ., Yokohama, 223, Japan

Tetrahedron Letters (1990), 31(5), 709-12 CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

OS CASREACT 113:131820

GΙ

SO

AB Oleandolide (I) has been synthesized by coupling the C(1)-C(7) and C(8)-C(14) segments which are enantiospecifically derived from Me  $\alpha$ -L- and D-rhamnosides, resp.

IT 129413-26-9P 129446-68-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 129413-26-9 CAPLUS

CN 7-Octenoic acid, 2,4,6-trimethyl-3,5-bis(phenylmethoxy)-, 6-(dimethoxyphosphinyl)-5-hydroxy-1,2,4-trimethyl-3-(phenylmethoxy)hexyl ester, [1R-[1R\*(2R\*,3S\*,4R\*,5S\*,6S\*),2S\*,3R\*,4S\*,5R\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 129446-68-0 CAPLUS

CN 7-Octenoic acid, 2,4,6-trimethyl-3,5-bis(phenylmethoxy)-, 6-(dimethoxyphosphinyl)-5-hydroxy-1,2,4-trimethyl-3-(phenylmethoxy)hexyl ester, [1R-[1R\*(2R\*,3S\*,4R\*,5S\*,6R\*),2S\*,3R\*,4S\*,5R\*]]- (9CI) (CA INDEX

Absolute stereochemistry.

L7 ANSWER 37 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1990:419973 CAPLUS <<LOGINID::20080519>>

DN 113:19973

OREF 113:3377a,3380a

TI Activities of native and tyrosine-69 mutant phospholipases A2 on phospholipid analogs. A reevaluation of the minimal substrate requirements

AU Kuipers, Oscar P.; Dekker, Nicolaas; Verheij, Hubertus M.; De Haas, Gerard

CS Dep. Biochem., Univ. Utrecht, Utrecht, NL-3508 TB, Neth.

SO Biochemistry (1990), 29(25), 6094-102 CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

AΒ The role of tyrosine (Tyr)-69 of porcine pancreatic phospholipase A2 in substrate binding was studied with the help of proteins modified by site-directed mutagenesis and phospholipid analogs with a changed head-group geometry. Two mutants were used containing phenylalanine (Phe) and lysine (Lys), resp., at position 69. Modifications in the phospholipids included introduction of a S atom at the P atom (thionophospholipids), removal of the neg. charge at the P atom (phosphatidic acid di-Me ester), and reduction (phosphonolipids) or extension (diacylbutanetriol choline phosphate) of the distance between the P atom and the acyl ester bond. Replacement of Tyr-69 by Lys reduced enzymic activity, but the mutant enzyme retained both the stereospecificity and positional specificity of native phospholipase A2. The Phe-69 mutant not only hydrolyzed the Rp isomer of thionophospholipids more efficiently than the wild-type enzyme, but the Sp thiono isomer was hydrolyzed too, although at a low (.apprx.4%) rate. Phosphonolipids were hydrolyzed by native phospholipase A2 .apprx.7-fold more slowly than natural phospholipids, with retention of positional specificity and a (partial) loss of stereospecificity. The di-Me ester of phosphatidic acid was degraded efficiently in a Ca2+-dependent and positional-specific way by native phospholipase A2 and by the mutants, indicating that a neq. charge at the P atom is not an absolute substrate requirement. The activities on the phosphatidic acid di-Me ester of native enzyme and the Lys-69 mutant were lower than those on the corresponding lecithin, in contrast to the Phe-69 mutant, which had equal activities on both substrates. The data suggested that in porcine pancreatic phospholipase A2 fixation of the phosphate group is achieved both by an interaction with the phenolic OH of Tyr-69 and by an interaction with the Ca2+. In mutant Y69K, the  $\epsilon\textsc{-NH2}$  group can play a role similar to that of the Tyr OH group in native PLA2. smaller side-chain of the Y69F mutant could interact with more bulky head-groups, allowing for relatively high enzymic activities on modified phospholipids. On the basis of these results, a reevaluation of the

minimal substrate requirements of phospholipase A2 is presented.

IT 127572-40-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acylation of)

RN 127572-40-1 CAPLUS

L7 ANSWER 38 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1989:457412 CAPLUS <<LOGINID::20080519>>

DN 111:57412

OREF 111:9739a,9742a

TI Preparation of chiral fosfomycin intermediates

IN Castaldi, Graziano; Giordano, Claudio

PA Zambon Group S.p.A., Italy

SO Eur. Pat. Appl., 23 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

T 1711 4 O 14 T												
	PA:	TENT NO.		KIND		DATE		AP	PLICAT	DATE		
					_							
ΡI	ΕP	299484		A1		1989	0118	EP	1988-	19880714		
	ΕP	299484		B1 19911009								
		R: AT, E	E, CH,	DE,	ES	, FR,	GB,	GR, I	T, LI,	LU, N	L, SE	
	US	4937367		Α		1990	0626	US	1988-	217976		19880712
	ΑT	68188		T		1991	1015	AT	1988-	111335		19880714
	ES	2037770		Т3		1993	0701	ES	1988-	111335		19880714
	JΡ	01104085		Α		1989	0421	JP	1988-	177950		19880715
PRAI	ΙT	1987-21303		A		1987	0715					
	ΙT	1987-23125	1	А		1987	1221					
	ΕP	1988-11133	5	А		1988	0714					

OS MARPAT 111:57412

S, S-MeCH(OH)CH(OSO2R1)P(O)(OR2)(OR3) (I; R1 = alkyl, aryl, arylalkyl, D-AΒ or L-camphoryl; R2, R3 = H, alkyl, PhCH2, Na), useful as fosfomycin intermediates, were prepared in several steps from S-RCO2CHMeCOX (II) [R = alkyl, alkoxy, (substituted) Ph, PhCH2, naphthyl; X = Cl, Br, alkoxy, alkylsulfonyloxy, alkoxycarbonyloxy] and Me3SiOP(OR2)(OR3) (III). Me3SiOP(OMe)2 was added to 2S-acetoxypropionyl chloride (preparation given) over 15 min at 15° and the mixture was kept at 15° for 30 min to give di-Me 2S-acetoxypropionylphosphonate. The latter in PhMe was treated with Bu4NBH4 in PhMe to give a 75:25 mixture of 1S,2S- and 1R,2S-di-Me 2-acetoxy-1-hydroxypropylphosphonate. The 1S,2S-isomer in CH2Cl2/pyridine at 0° was treated with MeSO2Cl to give di-Me 1S, 2S-2-acetoxy-1-mesyloxypropylphosphonate. The latter was refluxed 6 h with MeSO3H in MeOH to give 1S,2S-2-hydroxy-1-mesyloxypropylphosphonate, which was converted to fosfomycin di-Me ester upon treatment with K2CO3 in MeOH.

IT 121467-14-9P

RL: SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP

Absolute stereochemistry.

Absolute stereochemistry.

Na

RN 121467-11-6 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 2-hydroxy-1-methyl-2-phosphonoethyl ester, monosodium salt,  $[R-(R^*,S^*)]-$  (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Na

RN 121467-12-7 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 2-(dimethoxyphosphinyl)-2-hydroxy-1-methylethyl ester,  $[R-(R^*,S^*)]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 121467-13-8 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxypropyl]-, dimethyl ester,  $[R-(R^*,S^*)]-$  (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 121382-43-2P 121382-44-3P 121382-45-4P

121467-10-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as fosfomycin intermediate)

RN 121382-43-2 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 2-hydroxy-1-methyl-2-phosphonoethyl ester, monosodium salt,  $[S-(R^*,R^*)]-(9CI)$  (CA INDEX NAME)

Absolute stereochemistry.

Na

CN Propanoic acid, 2,2-dimethyl-, 2-(dimethoxyphosphinyl)-2-hydroxy-1-methylethyl ester,  $[S-(R^*,R^*)]-$  (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 121382-45-4 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxypropyl]-, dimethyl ester,  $[S-(R^*,R^*)]-(9CI)$  (CA INDEX NAME)

Absolute stereochemistry.

RN 121467-10-5 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxypropyl]-, monosodium salt,  $[R-(R^*,S^*)]-$  (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● Na

IT 121382-46-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for fosfomycin)

RN 121382-46-5 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxypropyl]-, bis(1,1-dimethylethyl) ester,  $[S-(R^*,R^*)]-(9CI)$  (CA INDEX NAME)

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L7 ANSWER 39 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
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AN 1989:423836 CAPLUS <<LOGINID::20080519>>

DN 111:23836

OREF 111:4161a,4164a

TI Phosphonolipids. 2.  $\alpha\textsc{-Hydroxyphosphonolipid}$  analogs of phosphatidic acid

AU Schwartz, Patricia Waters; Tropp, Burton E.; Engel, Robert

CS Queens Coll., City Univ. New York, Flushing, NY, 11367, USA

SO Chemistry and Physics of Lipids (1988), 49(1-2), 131-4 CODEN: CPLIA4; ISSN: 0009-3084

DT Journal

LA English

GΙ

Nominally isosteric phosphonic acid analogs I (R = C9H19, C15H31) of phosphatidic acid have been synthesized wherein a hydroxyl group is incorporated at the site adjacent to the phosphonyl center. The incorporation of the hydroxyl group into these analogs provides a means by which the mol. can interact with solvent or an enzyme site in a manner similar to that of the natural phospholipid. Unshared electron pairs associated with the hydroxyl group can mimic the interactions of the ester oxygen of the natural materials. The capability for such interaction is absent from ordinary isosteric methylene analogs.

IT 121335-79-3P 121335-81-7P 121335-84-0P

121335-85-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and removal of iso-Pr groups from)

RN 121335-79-3 CAPLUS

CN Decanoic acid,  $1-[2-[bis(1-methylethoxy)phosphinyl]-2-hydroxyethyl]-1,2-ethanediyl ester, <math>[R-(R^*,S^*)]-(9CI)$  (CA INDEX NAME)

RN 121335-81-7 CAPLUS

CN Hexadecanoic acid,  $1-[2-[bis(1-methylethoxy)phosphiny1]-2-hydroxyethyl]-1,2-ethanediyl ester, <math>[R-(R^*,S^*)]-(9CI)$  (CA INDEX NAME)

Absolute stereochemistry.

RN 121335-84-0 CAPLUS

CN Decanoic acid,  $1-[2-[bis(1-methylethoxy)phosphinyl]-2-hydroxyethyl]-1,2-ethanediyl ester, <math>[S-(R^*,R^*)]-(9CI)$  (CA INDEX NAME)

Absolute stereochemistry.

RN 121335-85-1 CAPLUS

CN Hexadecanoic acid,  $1-[2-[bis(1-methylethoxy)phosphinyl]-2-hydroxyethyl]-1,2-ethanediyl ester, <math>[S-(R^*,R^*)]-(9CI)$  (CA INDEX NAME)

Absolute stereochemistry.

RN 121335-83-9 CAPLUS
CN Hexadecanoic acid, 1-(2-hydroxy-2-phosphonoethyl)-1,2-ethanediyl ester,
[R-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 121335-86-2 CAPLUS
CN Decanoic acid, 1-(2-hydroxy-2-phosphonoethyl)-1,2-ethanediyl ester,
 [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

RN 121335-87-3 CAPLUS

CN Hexadecanoic acid, 1-(2-hydroxy-2-phosphonoethyl)-1,2-ethanediyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me 
$$(CH_2)_{14}$$
 O O  $(CH_2)_{14}$  Me  $H_2O_3P$  S OH

L7 ANSWER 40 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1989:231726 CAPLUS <<LOGINID::20080519>>

DN 110:231726

OREF 110:38427a,38430a

TI Acetals with a phosphorus substituent in the alcohol portion

AU Gazizov, M. B.; Khairullin, R. A.

CS Kazan. Khim.-Tekhnol. Inst., Kazan, USSR

SO Zhurnal Obshchei Khimii (1988), 58(7), 1493-504

CODEN: ZOKHA4; ISSN: 0044-460X

DT Journal

LA Russian

OS CASREACT 110:231726

GΙ

$$(CH_2)_n \\ O \\ OCHR^5P(O)(OR^6)_2 \\ I \\ O \\ O \\ O \\ II$$

AB Treating CH2:CHOR (R = Et, Bu) with R1(R2O)P(Z)CR3R4OH (R1 = MeO, EtO, Me2CHO, PrO, Me, Et, Ph, BuO; R2 = Me, Et, Me2CH, Pr, Bu; R3 = H, Me, vinyl, 2-furyl; R4 = H, Me; Z = O, S) in the presence of HCl gave 60-98% R1(R2O)P(Z)CR3R4OCH(OR)Me. Cyclic analogs I (R5 = H, Me; R6 = Me, Et; n = 1, 0) were prepared in 79-96% yields by treating 3,4-dihydropyran or 2,3-dihydrofuran with (R6O)2P(O)CHR5OH and HCl. Reaction of MeCOCH2OH with (R7O)2PHO (R7 = Me, Et, Pr, Bu), followed by cyclization with (EtO)3CH gave 27-48% dioxolanes II (same R7).

IT 83367-75-3

RL: RCT (Reactant); RACT (Reactant or reagent) (intramol. cyclization of, dioxolane by)

RN 83367-75-3 CAPLUS

CN Phosphonic acid, [2-(1-ethoxyethoxy)-1-hydroxy-1-methylethyl]-, dibutyl ester (9CI) (CA INDEX NAME)

IT 83367-72-0P 83367-73-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and intramol. cyclization of, dioxolane by)

RN 83367-72-0 CAPLUS

CN Phosphonic acid, [2-(1-ethoxyethoxy)-1-hydroxy-1-methylethyl]-, dimethyl ester (9CI) (CA INDEX NAME)

RN 83367-73-1 CAPLUS

CN Phosphonic acid, [2-(1-ethoxyethoxy)-1-hydroxy-1-methylethyl]-, diethyl ester (9CI) (CA INDEX NAME)

IT 120678-82-2P

RN 120678-82-2 CAPLUS

CN Phosphonic acid, [3-(1-ethoxyethoxy)-1-hydroxy-1-methylpropyl]-, dimethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 41 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1988:630649 CAPLUS <<LOGINID::20080519>>

DN 109:230649

OREF 109:38137a,38140a

TI Preparation and formulation of alkoxyphosphonoguanines as antiviral agents

IN Reist, Elmer J.; Sturm, Priscilla A.

PA SRI International, USA

SO PCT Int. Appl., 63 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.				KIND	D	DATE	AP:	PLICATION NO.	DATE	
PI	WO	8805438 W: DE, GB,		JP,	A1 NL, S		9880728	WO	1987-US3446	 19871223	
		RW:	FR,	ΙT							
	NL	8720	745			А	1	9881201	NL	1987-20745	19871223
	DE	3790	883			ΤO	1	9881208	DE	1987-3790883	19871223
	EΡ	30949	91			A1	1	9890405	EP	1988-900934	19871223
		R:	FR,	ΙT							
	JΡ	0150	1864			Τ	1	9890629	JP	1988-501095	19871223
	GB	2209	338			Α	1	9890510	GB	1988-21380	19880912
	SE	88033	309			Α	1	9880919	SE	1988-3309	19880919
	US	5047	533			А	1	9910910	US	1990-469791	19900122
PRAI	US	1987	-547	1		Α	1	9870120			
	US	1983	-497	720		В2	1	9830524			
	US	1986	-828	231		В2	1	9860210			
	WO	1987	-US3	446		А	1	9871223			
OS MARPAT 109:230649											

GI For diagram(s), see printed CA Issue.

Title compds. BCH2OCHR1(CH2)nCHR2P(O)(OH)2 (I; B = purine base conjugated through the 9-position; R1 = H, Me, HOCH2 and its alkyl esters, halomethyl, N3CH2, NC; R2 = H, Me, HOCH2 and its alkyl esters, halomethyl, N3CH2, NC; HO and its alkyl esters; R2H = O; n = 0-5) and pharmaceutically acceptable acid addition salts, mono- and dibasic salts, mono- and diesters thereof, and II and pharmaceutically acceptable acid addition salts, monobasic salts and monoesters thereof, were prepared 6-Chloro-9-(3-diethylphosphono-1-propoxymethyl)guanine (preparation given) combined with 1H NaOH and was refluxed and lyophilized to give mono-Et I (B = 2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl; R1, R2 = H; n = 1) (III). In in vivo test in guinea pigs against HSV-1TK+, III in 1-2% (saturated solution)

vivo test in guinea pigs against HSV-1TK+, III in 1-2% (saturated solution) resulted in 0.9 number of lesions compared to 0.4% solution that resulted in 2.1

number of lesions compared to acyclovir (control) 1.0 number of lesions. IT 117611-21-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and condensation with silated aminochloropurine)

RN 117611-21-9 CAPLUS

CN Phosphonic acid, [4-(acetyloxy)-3-hydroxybutyl]-, diethyl ester (9CI) (CA

## INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{O} \\ | & | \\ \text{AcO-CH}_2\text{-CH-CH}_2\text{-CH}_2\text{-P-OEt} \\ | & | \\ \text{OEt} \end{array}$$

L7 ANSWER 42 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1983:612705 CAPLUS <<LOGINID::20080519>>

DN 99:212705

OREF 99:32743a,32746a

TI Antiinflammatory and antiarthritic pyrazolylethanephosphonates.

IN Biere, Helmut; Rufer, Clemens; Boettcher, Irmgard

PA Schering A.-G., Fed. Rep. Ger.

SO Ger. Offen., 19 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡI	DE 3203307	A1	19830728	DE 1982-3203307	19820127	
PRAI	DE 1982-3203307		19820127			
OS CASREACT 99:21270		: MARPAT	99:212705			
GI						

$$F \xrightarrow{N} \stackrel{R}{\longrightarrow} C1$$

AB Approx. 20 title compds. I [R = CH:C(OH)P(O)(OEt)2 (II), CH2CH(OH)P(O)(ONa)2, CH2C(NH2)P(O)(OH)2, etc.] were prepared Thus, 17.5 g 4-(p-chlorophenyl)-1-(p-fluorophenyl)-3-pyrazoleacetyl chloride in 100 mL THF was treated with 9.8 mL P(OEt)3 to give 83.4% II, which was hydrolyzed to give 74.2% I [R = CH:C(OH)P(O)(OH)2].

IT 87965-40-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 87965-40-0 CAPLUS

CN 1H-Pyrazole-3-acetic acid, 4-(4-chlorophenyl)-1-(4-fluorophenyl)-, 2,2-bis(diethoxyphosphinyl)-2-hydroxyethyl ester (CA INDEX NAME)

CN 1H-Pyrazole-3-acetic acid, 4-(4-chlorophenyl)-1-(4-fluorophenyl)-, 2-hydroxy-2,2-diphosphonoethyl ester (CA INDEX NAME)

RN 87973-45-3 CAPLUS

CN 1H-Pyrazole-3-acetic acid, 4-(4-chlorophenyl)-1-(4-fluorophenyl)-, 2-hydroxy-2,2-diphosphonoethyl ester, disodium salt (9CI) (CA INDEX NAME)

•2 Na

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L7
     ANSWER 43 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN
     1982:563104 CAPLUS <<LOGINID::20080519>>
ΑN
DN
     97:163104
OREF 97:27209a,27212a
ΤI
     2-Methyl-4-phosphorylated 1,3-dioxolanes
     Gazizov, M. B.; Galiullina, I. I.; Krasil'nikova, E. A.; Rodintseva, E. V.
ΑU
CS
     Kazan. Khim.-Tekhnol. Inst., Kazan, USSR
     Zhurnal Obshchei Khimii (1982), 52(6), 1434-5
SO
     CODEN: ZOKHA4; ISSN: 0044-460X
\mathsf{DT}
     Journal
LA
     Russian
     CASREACT 97:163104
OS
GΙ
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Ι

CN Phosphonic acid, [2-(1-ethoxyethoxy)-1-hydroxy-1-methylethyl]-, dimethyl

ester (9CI) (CA INDEX NAME)

RN 83367-73-1 CAPLUS

CN Phosphonic acid, [2-(1-ethoxyethoxy)-1-hydroxy-1-methylethyl]-, diethyl ester (9CI) (CA INDEX NAME)

RN 83367-74-2 CAPLUS

CN Phosphonic acid, [2-(1-ethoxyethoxy)-1-hydroxy-1-methylethyl]-, dipropyl ester (9CI) (CA INDEX NAME)

RN 83367-75-3 CAPLUS

CN Phosphonic acid, [2-(1-ethoxyethoxy)-1-hydroxy-1-methylethyl]-, dibutyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 44 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1977:480068 CAPLUS <<LOGINID::20080519>>

DN 87:80068

OREF 87:12713a,12716a

TI Isosteres of natural phosphates. 6. The preparation and properties of lysophosphotidic acid

AU Tang, Ju-Chao; Tang, Chu-Tay; Tropp, Burton E.; Engel, Robert

CS Queens Coll., City Univ. New York, Flushing, NY, USA

- SO Chemistry and Physics of Lipids (1977), 19(2), 99-106 CODEN: CPLIA4; ISSN: 0009-3084
- DT Journal
- LA English

AB Phosphonic acid analogs of lysophosphatidic acid were synthesized. The racemic isosteric analogs, 4-acyloxy-3-hydroxybutyl-1-phosphonic acids, of lysophosphatidic acid were prepared by both catalytic and hydride redns. of the 4-acyloxy-3-oxobutyl-1-phosphonic acids, a general method for the preparation of the latter having been reported previously. The lysophosphatidic acids are substrates for lysophosphatidic acid acyltransferase, and may be acylated chemical to yield phosphotidic acids. The latter reaction is of use in the preparation of differentially acylated phosphatidic acids.

IT 64032-88-8P 64032-89-9P

RN 64032-88-8 CAPLUS

CN Hexadecanoic acid, 2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

RN 64032-89-9 CAPLUS

CN Octadecanoic acid, 2-hydroxy-4-phosphonobutyl ester (CA INDEX NAME)

L7 ANSWER 45 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1977:55638 CAPLUS <<LOGINID::20080519>>

DN 86:55638

OREF 86:8881a,8884a

TI Phosphorus-containing carbohydrates, XV. Perkow reaction with  $\alpha\text{-acyloxy}$  keto sugars for the synthesis of enol phosphates and their reactions

AU Thiem, Joachim; Rasch, Dieter; Paulsen, Hans

CS Inst. Organ. Chem. Biochem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.

SO Chemische Berichte (1976), 109(11), 3588-97 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

GΙ

The Perkow reaction of 1,3,4,5,6-penta-O-acetyl-keto-D-fructose with P(OMe)3 gave the enol phosphates I and II, which hydrolyzed to 1-deoxy-D-fructose and 3-deoxy-D-erythro-hexulose, resp. Similarly 2,3,4,5,6-penta-O-acetyl-aldehydo-D-glucose gave the enol phosphate III, which hydrolyzed to 2-deoxyglucose. The Perkow reaction of IV (RR1 = 0, R2 = H, R3 = OBz; R = OBz, R1 = H, R2R3 = O) with subsequent hydrolysis gave IV (RR1 = 0, R2 = R3 = H; R = R1 = H, R2R3 = O), resp.

IT 61521-44-6P 61521-46-8P

RN 61521-44-6 CAPLUS

CN D-Glucitol, 1-C-(dimethoxyphosphinyl)-, 2,3,4,5,6-pentaacetate, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 61521-46-8 CAPLUS

CN D-Glucitol, 1-C-(dimethoxyphosphinyl)-, 2,3,4,5,6-pentaacetate, (S)- (9CI) (CA INDEX NAME)

L7 ANSWER 46 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1976:543296 CAPLUS <<LOGINID::20080519>>

DN 85:143296

OREF 85:22973a,22976a

TI Substituted ethane diphosphonic acids, salts, and esters

IN Kerst, Al F.

PA Monsanto Co., USA

SO U.S., 15 pp. Division of U.S. 3,899,528.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 5

ran.cni 5						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 3962318	A	19760608	US 1975-560837	19750321	
1	US 3705191	A	19721205	US 1970-27988	19700413	
1	US 3833690	A	19740903	US 1972-283147	19720823	
1	US 3899528	A	19750812	US 1974-463224	19740423	
PRAI	US 1970-27988	А3	19700413			
1	US 1972-283147	A3	19720823			
1	US 1974-463224	А3	19740423			
GI						

AB 1CH2CR2[P(0)(OR)2]2 (I, R = H, Na, K, Zn, NH4, Et, Bu, Ph, etc.; R1, R2 = OH, CN, NH2, NEt2, SEt, CO2Et, etc.) were prepared by deoxiranization of II with H2O, amines, mercaptans etc. Thus, heating II (R = H) with H2O at  $90^{\circ}$  3 hr gave I (R = H, R1 = R2 = OH). I have sequestering and flame retardant properties.

IT 34619-93-7P 34619-94-8P

RN 34619-93-7 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)

RN 34619-94-8 CAPLUS

CN Phosphonic acid, [1-(acetyloxy)-2-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)

L7 ANSWER 47 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1976:524141 CAPLUS <<LOGINID::20080519>>

DN 85:124141

OREF 85:19933a,19936a

TI Substituted ethane diphosphonic acids and salts and esters

IN Kerst, Al F.

PA Monsanto Co., USA

SO U.S., 13 pp. Division of U.S. 3,705,191.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	US 3957858	 A	 19760518	US 1972-283146	19720823
	US 3705191	A	19721205	US 1970-27988	19700413
	NL 7104745	A	19711015	NL 1971-4745	19710408
	FR 2089481	A5	19720107	FR 1971-12737	19710409
	ES 390099	A1	19730601	ES 1971-390099	19710412
	CA 986944	A1	19760406	CA 1971-110062	19710412
	BE 765633	A1	19711013	BE 1971-102103	19710413
	GB 1329879	A	19730912	GB 1971-26858	19710419
	US 3816518	A	19740611	US 1972-234328	19720313
	US 3846482	A	19741105	US 1972-283019	19720823
	US 3846483	A	19741105	US 1972-283115	19720823
	US 3890378	A	19750617	US 1972-283114	19720823
PRAI GI	US 1970-27988	A3	19700413		

AB RCH2CR1[P(0)(OR2)2]2 (I, R, R1 = OH, NH2, C1, CN, Bz, SEt, etc.; R2 = H, Na, alkyl) (.apprx.32 compds.) were prepared mainly by deoxiranization of epoxyethanediphosphonates. Thus, hydrolysis of II with H2O at  $90^{\circ}$  for 3 hr gave I (R = R1 = OH, R2 = H). I have sequestering and fire retardant properties in textiles.

IT 34619-93-7P 34619-94-8P

RN 34619-93-7 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)

RN 34619-94-8 CAPLUS

CN Phosphonic acid, [1-(acetyloxy)-2-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)

L7 ANSWER 48 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1976:421611 CAPLUS <<LOGINID::20080519>>

DN 85:21611

OREF 85:3541a,3544a

TI Substituted ethanediphosphonic acids and salts

IN Kerst, Al F.

PA Monsanto Co., USA

SO U.S., 13 pp. Division of U.S. 3,833,690.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 5

L WIN .	CNIJ					
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡI	US 3944599	A	19760316	US 1973-422227	19731206	
	US 3705191	A	19721205	US 1970-27988	19700413	
	US 3833690	A	19740903	US 1972-283147	19720823	
PRAI	US 1970-27988	А3	19700413			
	US 1972-283147	<b>A</b> 3	19720823			
GI						

AB Cleavage of epoxides I (R = R1 = H, Et; R = H, R1 = Na, Ph) with acids, alcs., amines, mercaptans, etc. gave .apprx.30 R2CH2CR3[P(O)(OR)(OR1)]2 (II, R = R1 = H, Et, NH4, K; R = H, R1 = Na, Ph; R2, R3 = OH, NH2, C1,

OAc, CN, OBz, OPr, SEt, etc.). Thus, 100 g I (R = R1 = H) in 500 ml CCl4 was treated with HCl gas to give ClCH2C(OH)[P(O)(OH)2]2 and HOCH2CCl[P(O)(OH)2]2. II were sequestrants and flame retardants for cotton textiles.

IT 34619-93-7P 34619-94-8P

RN 34619-93-7 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)

RN 34619-94-8 CAPLUS

CN Phosphonic acid, [1-(acetyloxy)-2-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)

L7 ANSWER 49 OF 58 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1976:180394 CAPLUS <<LOGINID::20080519>>

DN 84:180394

OREF 84:29243a,29246a

TI Substituted ethane diphosphonic acids, salts, and esters

IN Kerst, Al F.

PA Monsanto Co., USA

SO U.S., 13 pp. Division of U.S. 3,705,191.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 5

PATENT NO.		NO.	KIND	DATE	API	PLICATION NO.	DATE	
	ΡI	US 3940	436	A	19760224	US	1972-283251	19720823
		US 3705	191	A	19721205	US	1970-27988	19700413
		NL 7104	745	A	19711015	NL	1971-4745	19710408
		FR 2089	481	A5	19720107	FR	1971-12737	19710409
		ES 3900	99	A1	19730601	ES	1971-390099	19710412
		CA 9869	44	A1	19760406	CA	1971-110062	19710412
		BE 7656.	33	A1	19711013	BE	1971-102103	19710413
		GB 1329	879	A	19730912	GB	1971-26858	19710419
		US 3816	518	A	19740611	US	1972-234328	19720313
		US 3846	482	A	19741105	US	1972-283019	19720823
		US 3846	483	A	19741105	US	1972-283115	19720823
		US 3890.	378	A	19750617	US	1972-283114	19720823
	PRAI	US 1970	-27988	A3	19700413			

AB Epoxyethanediphosphonate I (R = H, Me, Et, Na) with water, amines, acids, alcs., mercaptans, etc. gave .apprx.15 R1CH2C(OH)[P(O)(OR)2]2 (R = same as above, R1 = OH, NH2, CN, SO3H, OPr, CO2Et, OPh, SEt, etc.). Thus, 0.38 mole I (R = Me) was refluxed 20 hr with 0.40 mole sodium or potassium cyanide in 400 ml MeCN to give H2C(CN)C(OH)[P(O)(OMe)2]2. The compds. prepared were sequestering agents and fireproofing agents for cotton textiles.

IT 34619-93-7P 34619-94-8P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 34619-93-7 CAPLUS

CN Phosphonic acid, [2-(acetyloxy)-1-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)

RN 34619-94-8 CAPLUS

CN Phosphonic acid, [1-(acetyloxy)-2-hydroxyethylidene]bis- (9CI) (CA INDEX NAME)